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Outdoor Smog Chamber Experiments To Test Photochemical Models: Phase II

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16. ABSTRACT

The smog chamber facility of the University of North Carolina was used to provide experimental data for developing and testing kinetic mechanisms of photochemical smog formation. In this study, 128 pairs of experiments were performed using NO_x and various hydrocarbons and hydrocarbon mixtures. The experiments performed during this three-year project have been added to the existing UNC data base for model testing, bringing the total number of pairs of experiments to 346. This report presents an organizational scheme for these 346 experiments. This scheme enables users of the data to readily access specific portions of the data set. The report also contains guidance to modelers about which experiments should be simulated to test various aspects of the models and what order the experiments should be simulated in.

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Abstract

The purpose of this project was to provide a database that modelers could use to develop new, improved mechanisms for use in urban air quality control models such as EKMA. One hundred and twenty eight outdoor smog chamber experiments were performed during the three years of this project. These have been added to the existing UNC database for photochemical mechanism validation and testing, bringing the total number of dual-experiments in the database to 345.

This report presents an organizational scheme for these 345 experiments. It uses six general attributes of each experiment to classify runs; these are:

- class of run, *e.g.* characterization, chemical test;
- experimental conditions, *e.g.* large or normal dilution, initial or continuous injection of reactants, HC-type, initial concentrations;
- experimental series, *e.g.* similar side-by-side conditions;
- quality, *e.g.* runs are graded on a scale of 0 to 9;
- processing status, *e.g.* form in which data are available;
- project that produced the data.

Experimental series form a major organizational basis. Two types of series were used: those based on the side-by-side conditions and those based on some chemical characteristic. All 345 runs fit into one of seven general side-by-side series:

- Matched Conditions—Both sides the same;
- Relative Reactivity—Comparison of different chemical systems;
- Substitution—Same total carbon with new species replacing some carbon on one side;
- Addition—All species on both sides the same except for additional carbon added to one side;
- Delta Concentration—Carbon or nitrogen concentration different on two sides;
- Static vs. Dynamic—One side is static, the other has large dilution, continuous injection, or both.

In addition, there are five series for characterization experiments. Finally, each run can appear in two other series from a set of five types, such as hydrocarbon class, or mixture representation.

Examples of selecting runs to test mechanisms for explicit toluene chemistry, dynamic operating conditions, and EKMA-type mechanism testing are given and discussed. Recommendations for how to use the side-by-side nature of the UNC chamber are given throughout the discussion.

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Michael Gery, Ph.D. student, designed and performed not only the CSTR aromatic experiments that are frequently cited herein, he also performed some of the aromatic chamber runs and he identified many aromatic reaction products on the site GC systems using MS. Figure 2 was drawn by Michael.

1

Introduction

Background

Role of Models in the Regulatory Process

Photochemical kinetics reaction models, which integrate diverse kinetics information into a unified description of urban atmospheric chemistry, are central components in the U.S. Environmental Protection Agency's (EPA) method for computing control requirements for organic emissions needed to meet Federal Air Quality Standards for ozone.[1]

State and local control officials are expected to use these models in a variety of situations to estimate control requirements. Guidance for the use of even the simplest models of this type can be quite complex.[2]

Development of Models

Models are of necessity simpler than the processes being modeled. This simplicity is achieved by the use of three techniques: generalization, deletion, and distortion.

In the generalization process, individual aspects of the process being modeled are treated as if they were identical to reduce the number of items that must be included in the model. In the deletion process some aspects of the process are ignored entirely in the model. In the distortion process, the model representation is changed from an exact representation in some way to an inexact and incorrect representation. Each of these processes may be used deliberately by the modeler or they can occur unintentionally.

Model creators apply these three processes differently and therefore, although they might be describing the same real world situation, the descriptions produced are often different. When these different descriptions predict different outcomes in the same situation, at least one of the models may not be "well-formed".

Need To Test Model Representation

Kinetic models are constructed mainly from theory and laboratory data derived by examining a few reactions at a time. In constructing the mechanisms, modelers hope to include all the important reactions, to leave out the non-essential reactions, and to generalize the complex free radical chemistry to provide an adequate, yet tractable description of the atmospheric chemistry of volatile organic compounds (VOC) and oxides of nitrogen (NO_x).

To determine the adequacy of such descriptions, mechanisms must be tested in situations similar to those in which the models are to be applied, and ideally, in situations in which the chemistry is the primary process affecting concentrations. Because of uncertainty in meteorology, ambient data such as that obtained in the EPA's Regional Air Pollution Study (RAPS) provide, at most, an ambiguous test situation. A useful but poor diagnostic test situation is provided by merely running the models through the same control scenario and comparing the predictions. If the predictions are different, clearly one or more of the models is inadequate in some manner, but which one? Ultimately, smog chamber data must provide mechanism test conditions to determine the adequacy of the chemical representation. These data, however, are not without their problems.

A mechanism comparison study conducted by Jeffries *et al.*,[3] demonstrated that although certain chemical reaction mechanisms could predict the outcomes of a large set of smog chamber experiments within the uncertainty of the data, these same mechanisms gave significantly different descriptions of the urban atmosphere. In particular, they differed greatly in the predicted magnitude of the change in ozone for a change in hydrocarbon at the same level of NO_x ($\Delta O_3/\Delta HC$), an important measure in urban control requirement calculations.

Subsequent studies and comparisons have been performed in an effort to understand why mechanism predictions differ.[4,5,6,7] These suggest that, among other things, small differences in how species are represented, or the omission of a species, can lead to relatively large differences in O_3 predictions. The studies do not, however, suggest which mechanism is the more correct one. This is because these studies did not systematically compare the mechanism predictions against a large range of data encompassing the range of conditions likely to occur in an urban control situation.

Model Testing Domain

Hierarchy of Species

Whitten, in a review of current knowledge of smog chamber chemistry,[8] described the concept of a "hierarchy" of chemical species based on the number of HC/NO_x systems in which the species occur, with the most ubiquitous species occupying the lowest levels. Using existing kinetic information, a complete hierarchy of species can be produced. Figure 1 is a slightly more detailed version of the schematic produced by Whitten.

Inorganic Species

The most common species are the inorganic species containing nitrogen, oxygen, and hydrogen since they occur in all HC/NO_x systems; these species appear at the bottom of the hierarchy (see Figure 1). Many reactions of these species have been studied in detail and good kinetics information is available.[9] Table 1 shows selected reactions from the Atkinson, Lloyd, Winges mechanism.[10] The first 20 reactions are typical of the inorganic species reactions used in current models.

The next higher species, in terms of increasing complexity of the chemistry, is carbon monoxide (CO). CO can effect the conversion of the hydroxyl radical ($HO^{\cdot}$) to the hydroperoxy radical ($HO_2^{\cdot}$) (see reaction 21 in Table 1). Experiments can be run with and without added CO allowing the model's predictions of the effects of CO to be directly tested. Models should always be able to account for the effects of added CO.

Simple Aldehydes

The next higher species in the hierarchy is formaldehyde ($HCHO$). Formaldehyde is a more complex molecule than CO, although its reactions do not produce any other

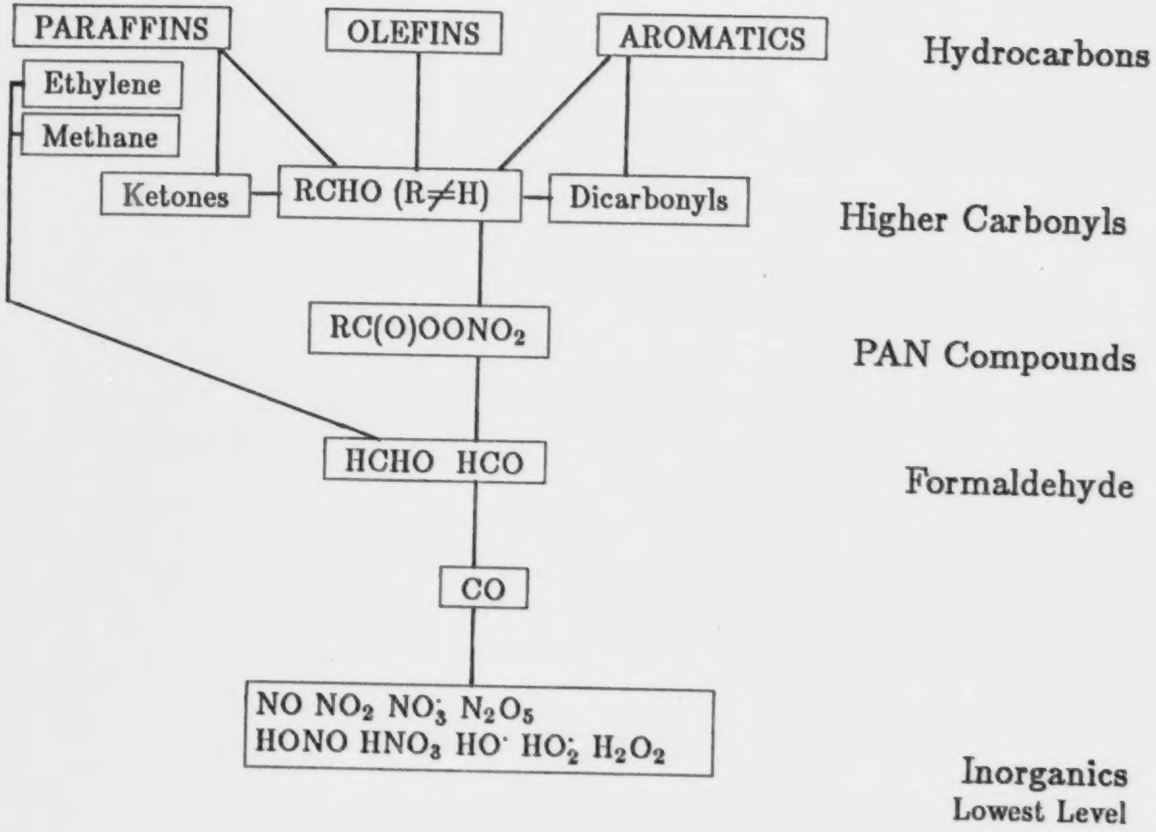
PARAFFINS
OLEFINS
AROMATICS
Hydrocarbons
Ethylene
Methane
Ketones
RCHO (R≠H)
Dicarbonyls
Higher Carbonyls
RC(O)OONO$_2$
PAN Compounds
HCHO HCO
Formaldehyde
CO
NO NO$_2$ NO$_3^{\cdot}$ N$_2$O$_5$
HONO HNO$_3$ HO$^{\cdot}$ HO$_2^{\cdot}$ H$_2$O$_2$
Inorganics
Lowest Level

Figure 1. Hierarchy of Species in Photochemical Mechanisms

Table 1.

THE ATKINSON ET AL. REACTION MECHANISM AS PRESENTED IN
TABLE A.2 OF THE LEONE AND SEINFELD REPORT PART 2
RENUMBERED AND RE-ORGANIZED BY JEFFRIES

```
(     INORGANIC REACTIONS     )

( 1) NO2 = NO + O3                       #1.0 /L;
( 2) NO + O3 = NO2                       #3355.7 @-1450;

( 3) NO2 + O3  = NO3                     #177.9 @-2450;
( 4) NO  + NO3 = 2.00*NO2                #28188;
( 5)       NO3 = 0.30*NO + 0.70*NO2 + 0.70*O3 #15.5 /L;
( 6) NO2 + NO3 = N2O5                    #104027 @-1100;
( 7)      N2O5 = NO2 + NO3               #3.5E18 @-12280;
( 8)      N2O5 = 2.00*HNO3               #4.46E-6 /W;

( 9)        O3 = 2.00*OH                 #2.3E-8 /W /L;

(10) OH  + NO = HONO                     #9796.9;
(11)     HONO = OH + NO                  #0.17 /L;

(12) OH  + NO2 = HNO3                    #16891;

(13) HO2 + NO  = OH + NO2                #12416;

(14) HO2 + NO2 = HO2NO2                  #1689;
(15)    HO2NO2 = HO2 + NO2               #7.8E15 @-10420;

(16) HO2 + HO2 = H2O2                    #114.09 @1100;
(17) HO2 + HO2 = H2O2                    #6.53E-10 @5800 /W;
(18)      H2O2 = 2.00*OH                 #7.1E-4 /L;

(19) OH  + O3 = HO2                      #2349 @-940;
(20) HO2 + O3 = OH                       #16.11 @-580;

(21) OH  + CO = HO2                      #436.2;
```

Table 1. cont.

```
( FORMALDEHYDE CHEMISTRY  )

(22) HCHO = 2.00*HO2 + CO                   #3.1E-3 /L;
(23) HCHO = CO                              #3E-3 /L;

(24) OH + HCHO = HO2 + CO                   #14765;

( ACETALDEHYDE CHEMISTRY )

(25)       CCHO = COO + HO2 + CO            #6E-4 /L;

(26) OH  + CCHO = CCO3                      #10067 @250;
(27) CCO3 + NO  = NO2 + COO                 #10403;
(28) CCO3 + NO2 = PAN                       #7047;
(29)        PAN = CCO3 + NO2                #1.2E18 @-13543;

(30) COO + NO = HCHO + HO2 + NO2            #10403;


( OLEFIN CHEMISTRY )

(49) OH + ETHENE   = -1.00*NO + NO2 + HO2 + 2.00*HCHO         #3255 @380;
(50) OH + PROPENE  = -1.00*NO + NO2 + HO2 + HCHO + CCHO       #6040 @540;

(52) O3 + ETHENE   = HCHO + 0.40*CH2DIOX + 0.40*CO + 0.12*HO2
                                                           #14.09 @-2560;
(53) O3 + PROPENE  = 0.50*HCHO + 0.50*CCHO + 0.20*CH2DIOX + 0.20*ETHDIOX
                     + 0.30*CO + 0.20*HO2 + 0.10*OH + 0.20*COO
                                                           #10.40 @-1900;
(55) CH2DIOX + NO  = HCHO + NO2              #10403;
(56) CH2DIOX + NO2 = HCHO + NO3              #1040;
(57)       CH2DIOX = (PRODUCT1)              #5.03E-3 /W;
(58) ETHDIOX + NO  = CCHO + NO2              #10403;
(59) ETHDIOX + NO2 = CCHO + NO3              #1040;
(60)       ETHDIOX = (PRODUCT2)              #5.03E-3 /W;
```

Table 1. cont.

```
KEY ::
        #  -- rate constant at 300 deg K or A-factor
        @  -- activation energy
        /L -- reaction depends upon light
        /W -- reaction depends upon water
        ;  -- end of reaction
       ( ) -- comments

UNITS :: PPM and MINS
```

significant organic species, only CO and $HO_2^\cdot$. In addition, formaldehyde ultimately occurs as a product in the reactions of every other organic species. Because the decomposition of $HCO^\cdot$ to produce $H^\cdot$ (and subsequently $HO_2^\cdot$) and CO is essentially an exclusive pathway,[9] there is no peroxy formyl nitrate species (HC(O)OO) to complicate the formaldehyde chemistry. Further, $HCO^\cdot$ and $H^\cdot$ are generally omitted from mechanisms in favor of immediately creating $HO_2^\cdot$ and CO, as in the photolysis reaction shown in Table 1 (reaction 22). This an example of the deletion and distortion processes applied to model development. The other reactions generally used to model HCHO are reactions 23 and 24 in Table 1.

The next higher aldehyde, acetaldehyde (CH_3CHO), reacts to produce intermediate products that ultimately produce formaldehyde and other species. The reactions typically used to model CH_3CHO are numbers 25 to 30 in Table 1. The species represented as COO in the table is $CH_3O_2^\cdot$ and once again the intermediate species $CH_3O^\cdot$ has been omitted in favor of its most likely reaction products, HCHO and $HO_2^\cdot$. Because reaction 30 produces HCHO, all of the formaldehyde reactions must be included in a successful mechanism for acetaldehyde but not vice versa. This fact puts acetaldehyde (and other aldehydes) on a higher level of the species hierarchy than formaldehyde.

Acetaldehyde is also the first compound to produce a peroxyacyl nitrate (PAN). PAN should be on a level between acetaldehyde and formaldehyde. All of the reactions of PAN are needed to successfully model acetaldehyde. If pure PAN was used as the organic reactant, no acetaldehyde would be present, none would be formed, and only the PAN sub-set of the CH_3CHO reactions would be needed. The reactions of PAN, however, lead to the production of formaldehyde (by way of $CH_3O_2^{\cdot}$) and thus PAN appears between these two aldehydes in the species hierarchy shown in Figure 1.

Simple Olefins

Ethylene reactions produce formaldehyde as the one significant organic product. Being an olefin, however, ethylene introduces the new elements of both $HO^{\cdot}$ and O_3 attacks on the double bond to an already tested formaldehyde mechanism. Reactions 49, 52, and 55 to 57 in Table 1 are highly compressed forms of the reactions of ethylene. They show that, for the most part, each carbon in ethylene is converted to HCHO. Ethylene therefore should fall somewhere between the higher olefins and formaldehyde in the hierarchy. Notice that ethylene can be used to test the double bond chemistry without the complication created by the production of PAN and its reactions.

Not only do the reactions of propylene involve both $HO^{\cdot}$ and O_3 attacks on the double bond, these reaction also produce both formaldehyde and acetaldehyde. Thus, propylene needs all the chemistry discussed so far except the direct attack of $HO^{\cdot}$ and O_3 on ethylene. In addition, reactions 50, 53 and 55–60 in Table 1 are needed. Propylene (and other olefins), therefore, appear on a higher level of the species hierarchy than other species we have discussed.

Other Species

Paraffins introduce not only the direct attack of $HO^{\cdot}$ on the paraffin itself, but also ketone and organic nitrate chemistry. Other paraffin products include species already described, *i.e.* CH_3CHO, HCHO, $HO_2^{\cdot}$.

Aromatics are still poorly understood. A summary of recent experimental data for the reaction of toluene with $HO^{\cdot}$ is shown in Figure 2.[11] Direct attacks on the aromatic species by $HO^{\cdot}$ include both addition and abstraction pathways. Some of the addition pathways lead to the production of cresols. Some ring opening apparently also occurs. This gives rise to dicarbonyl products such as glyoxal and methyl-glyoxal. The magnitude of the ring-opening process is highly uncertain. The reactivity of aromatics in models is highly dependent upon the assumed magnitude

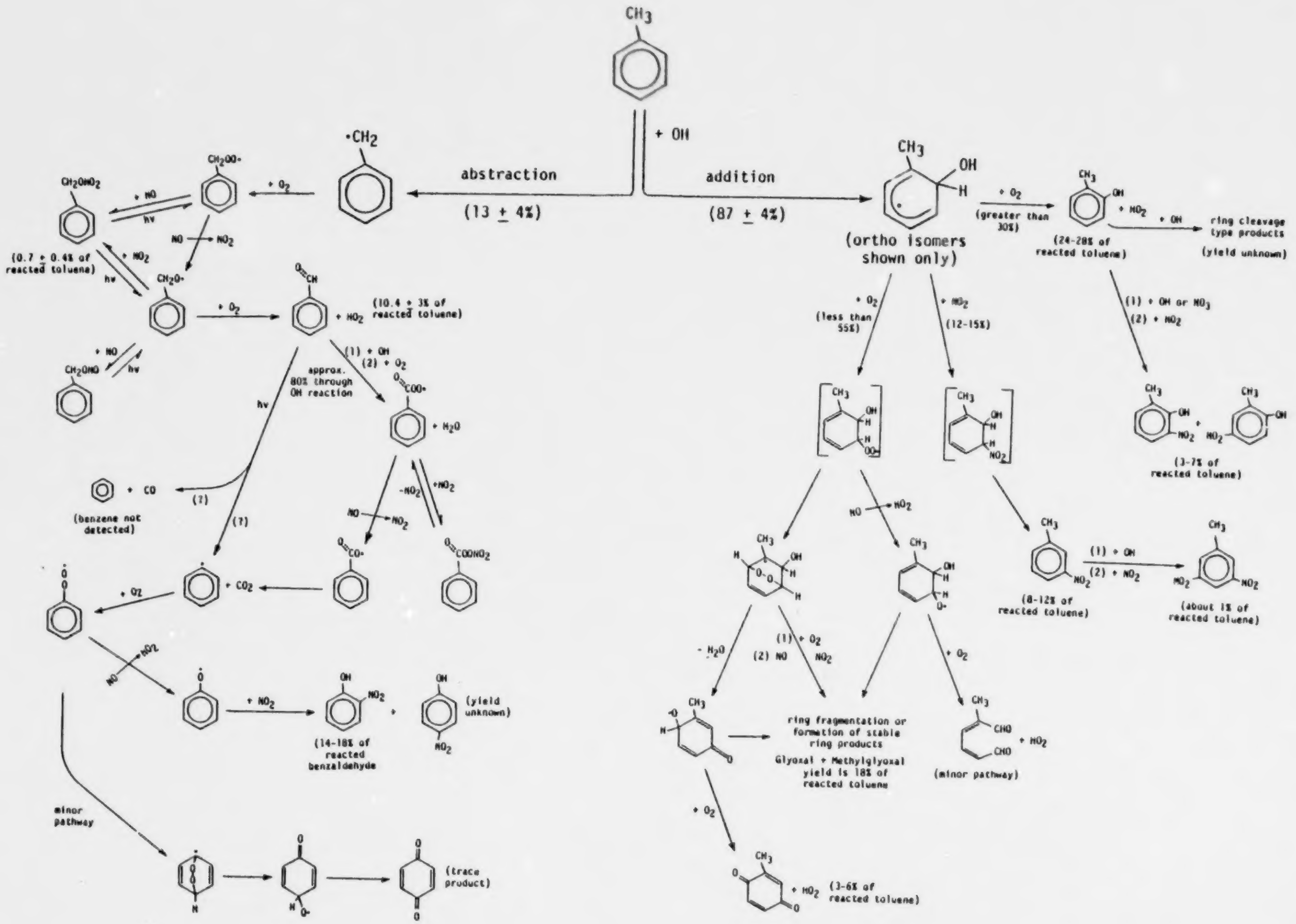
CH3
+ OH
abstraction
(13 ± 4%)
addition
(87 ± 4%)
•CH2
CH3
OH
H
(ortho isomers shown only)
+ O2
CH2OO•
CH2OHO2
+ NO
hv
NO → NO2
(0.7 ± 0.4% of reacted toluene)
+ NO2
hv
CH2O•
+ O2
+ HO2
(10.4 ± 3% of reacted toluene)
+ NO
hv
CH2ONO
(1) + OH
(2) + O2
approx. 80% through OH reaction
hv
+ H2O
-NO2
+NO2
NO → NO2
COONO2
CO•
COO•
+ CO
(?)
(benzene not detected)
(?)
+ CO2
+ O2
NO → NO2
+ NO2
OH
NO2
(14-18% of reacted benzaldehyde)
(yield unknown)
minor pathway
(trace product)
+ O2
(greater than 30%)
+ HO2
+ OH
ring cleavage type products
(yield unknown)
(24-28% of reacted toluene)
(1) + OH or NO3
(2) + NO2
(3-7% of reacted toluene)
+ O2
(less than 55%)
+ NO2
(12-15%)
NO → NO2
(8-12% of reacted toluene)
(1) + OH
(2) + NO2
(about 1% of reacted toluene)
- H2O
(1) + O2
(2) NO
NO2
+ O2
ring fragmentation or formation of stable ring products
Glyoxal + Methylglyoxal yield is 18% of reacted toluene
CHO
CHO
+ HO2
(minor pathway)
+ O2
+ HO2
(3-6% of reacted toluene)

Figure 2. Hydroxyl Radical-Toluene Reaction Scheme for the CSTR System.

of the processes that lead to dicarbonyl products. A number of aromatic experiments were performed in this project to test the aromatic portion of mechanisms.

The aromatic species are at the top of the hierarchy.

Guide for Experimentation

The hierarchical approach suggests that there is an ideal order in which a complete explicit mechanism should be developed and tested. Further, this approach suggests the type of smog chamber experiments needed: only one major new chemical process should be introduced into the model at a time and any changes that are necessary to the existing components of the mechanism must be verified by re-testing the lower hierarchical systems with the changed mechanisms. Whitten says:

> "Validating mechanisms in the stepwise order suggested by the use of hierarchical levels has two primary advantages: it clarifies the sources of uncertainty in simulations, and it reduces the probability that a complex mechanism for a large hydrocarbon contains compensating errors."[8]

Models Used to Design Experiments

As one proceeds higher in the hierarchy, the number of combinations of species that can be used to generate test conditions increases significantly. It is easier to produce a simulation than to run a smog chamber experiment. At some point, therefore, it is more productive to determine from the proposed mechanism some combination of species or conditions which should produce an unusual or unexpected result. That smog chamber experiment can then be run to verify the mechanism's predictions and thus support or refute the mechanism's description. This technique has been used by Whitten and Killus at System Applications Inc. (SAI) to predict conditions in which a propylene plus toluene experiment would produce less O_3 than the same concentration of propylene by itself. When we ran the experiment, the result was that predicted by SAI (Figure 3). This interaction, in which the model is used to suggest what experiment to perform, can quickly support or refute the validity of the model with a minimal number of experiments.

At some level of complexity in the development of models, it is no longer feasible to use an explicit species approach. Some generalizing and deletion process must be adopted. This leads to the creation of "lumped" or "surrogate" mechanisms. The hierarchical species approach, however, still provides a valuable strategy for testing

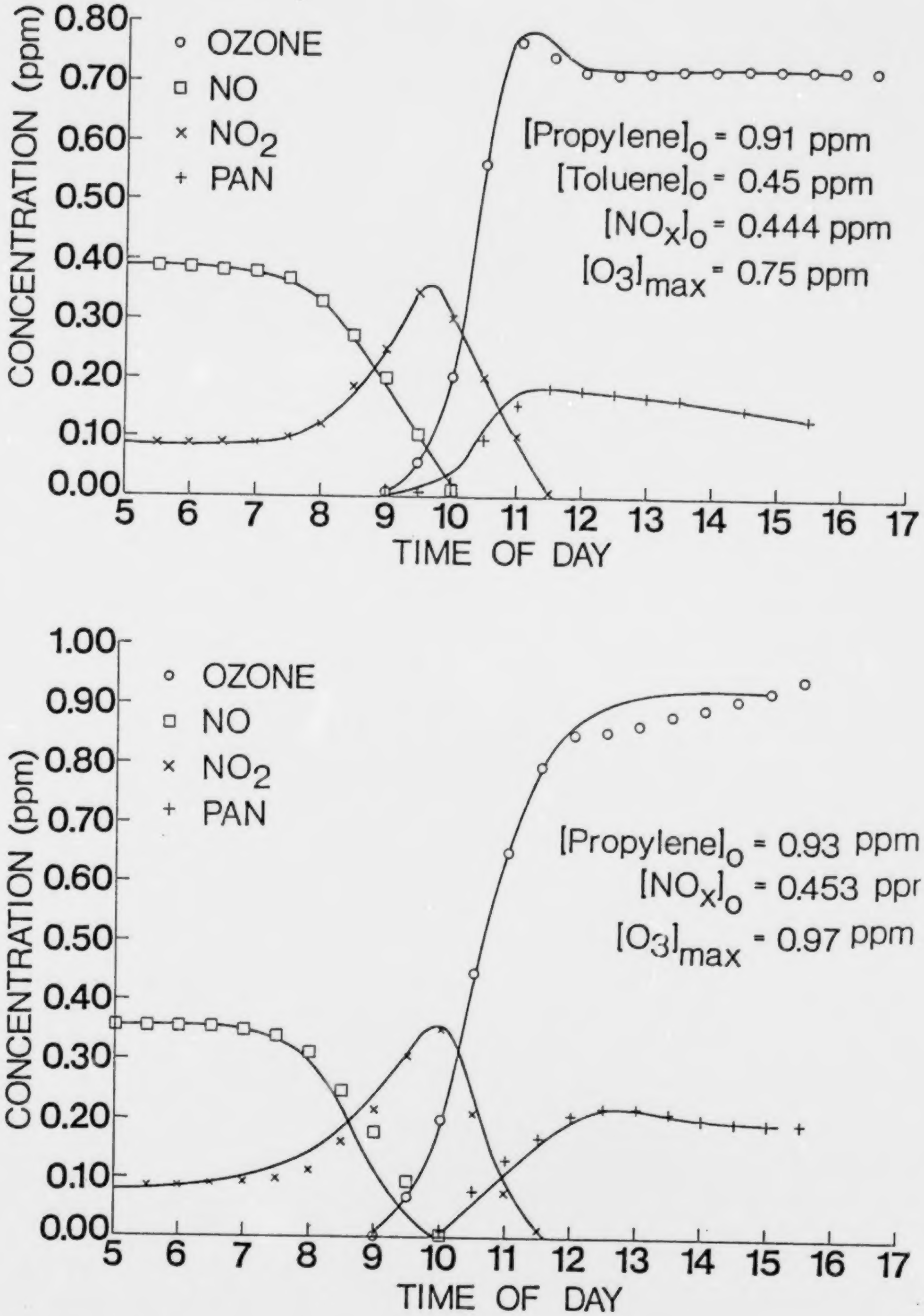

Figure 3. Effect of toluene addition to a matched propylene/NO_x system.

these condensed mechanisms: design experiments to test the mechanism from the "bottom up." That is, start with the simplest set of conditions that the mechanism is designed to simulate and increase the complexity of the experimental system one factor at a time.

Hierarchy of Experimental Conditions

The Whitten hierarchy described above stresses the role of species identity. Urban air pollution simulations, however, depend strongly on factors other than the identity of the reactants. The chemistry takes place in a highly dynamic environment including changing light intensity, changing temperature, constant injection of fresh reactant material, mixing of aged material from aloft, and large dilution of the reacting system. Ozone production is actually dominated by the fresh injection of NO and HC and by the dilution caused by the rise in mixing height.

It is not entirely safe to assume that because a mechanism successfully describes the changes to a few organic species in the relatively static environment of a traditional smog chamber, it will also provide an adequate description in a highly dynamic environment such as the urban atmosphere. The two situations tend to stress different parts of the chemical processes. The smog chamber tends to stress the product chemistry and the situation in which O_3 production is limited by lack of NO_x. The urban atmosphere tends to stress the initial reactant chemistry and is rarely NO_x-limited. As described above, our comparison study of four mechanisms tested with static smog chamber data demonstrated that mechanisms that could give reasonable fits to such smog chamber data could also give significantly different results in atmospheric applications.[3]

Thus a model validation database must also include experiments in which the processes of continuous injection and large dilution are considered. A combination of these two processes can also be described as an experimental hierarchy in which factors are introduced in a systematic fashion.

Table 2 illustrates four basic sets of chamber operating conditions that proceed stepwise from the standard smog chamber type experiment to conditions that simulate the urban environment. All conditions involve natural sunlight and ambient temperature. Two conditions involve no dilution, and two conditions involve large dilution. In each of these situations, reactants can either be introduced only initially or they can be introduced throughout the experiment. Within each of these four

Table 2. Hierarchy of Experimental Conditions to Simulate the Urban Environment

Outdoor chamber utilizing prevailing sunlight and near ambient temperatures simulates the urban light and temperature conditions; ambient humidity may be increased or reduced.

REACTANT INJECTION	NO DILUTION	LARGE DILUTION
	Dilution is minimized; dilution rates are $1.5x10^{-3}min^{-1}$, about 1% per hour.	Dilution is used to approximate various patterns of mixing height rises including: exponential (constant dilution rate), characteristic curve, and linear.
Initially Reactants are all injected before sunrise.	• Single organic compounds • Mixture of organic compounds o Simple mixtures: fewer than 6 species o Complex mixtures	• Single organic compounds • Mixture of organic compounds o Simple mixtures: fewer than 6 species o Complex mixtures
During Reactants are injected throughout the course of the experiment to simulate various emissions scenarios.	• Single organic compounds • Mixture of organic compounds ▹ Composition **constant** during injection o Simple mixtures: fewer than 6 species o Complex mixtures ▹ Composition **varying** during injection o Simple mixtures: fewer than 6 species o Complex mixtures	• Single organic compounds • Mixture of organic compounds ▹ Composition **constant** during injection o Simple mixtures: fewer than 6 species o Complex mixtures ▹ Composition **varying** during injection o Simple mixtures: fewer than 6 species o Complex mixtures

categories, the basic understanding of the chemistry of single compounds, simple mixtures, and complex mixtures can be tested.

A graphic example of Table 2 is provided by four experiments produced in this project; these are shown in Figure 4. Each of the four plots represents only one side of the dual outdoor chamber. Each shows the NO, NO_2, and O_3 profiles for a simple mixture of propylene, n-butane, and toluene. In the absence of reaction and dilution, all four experiments would have had essentially the same final concentrations of the reactants: 0.25 ppm NO_x and 2.6 ppmC of the mix. These four experiments alone represent a powerful test situation for urban-type mechanisms.

Matched Experimental Conditions

The uniqueness of the UNC dual chamber is also illustrated in Figure 4. The experiment of June 27 in the upper left-corner of the figure (*i.e.* static conditions), occurred under the same sunlight and temperature conditions as the experiment in the lower right-corner of Figure 4 (*i.e.* dynamic conditions). The data were taken with the same set of instruments at the same time. The same set of model inputs *must* be used for both simulations: the same set of temperature dependent rate constants, the same set of photolytic rates, the same 'adjustments' to measurements. Likewise, there are similar *static, and well understood—or easily-modelable*—chemical systems on the other side of the chamber for the other two dynamic runs shown in Figure 4. These side-by-side systems provide a powerful check on model assumptions and adjustments.

This side-to-side approach has proved so useful in creating clear examples of model test situations that we have used it extensively in producing the data described herein.

Range of Experiments Needed

One might consider only validating an urban mechanism at the most complex set of conditions: those in the lower right-corner of Table 2. Three factors argue against this approach:

- the large number of possible combinations of conditions in the urban-like simulations suggests that extremes in conditions may be the most feasible method of covering the range of conditions needed;

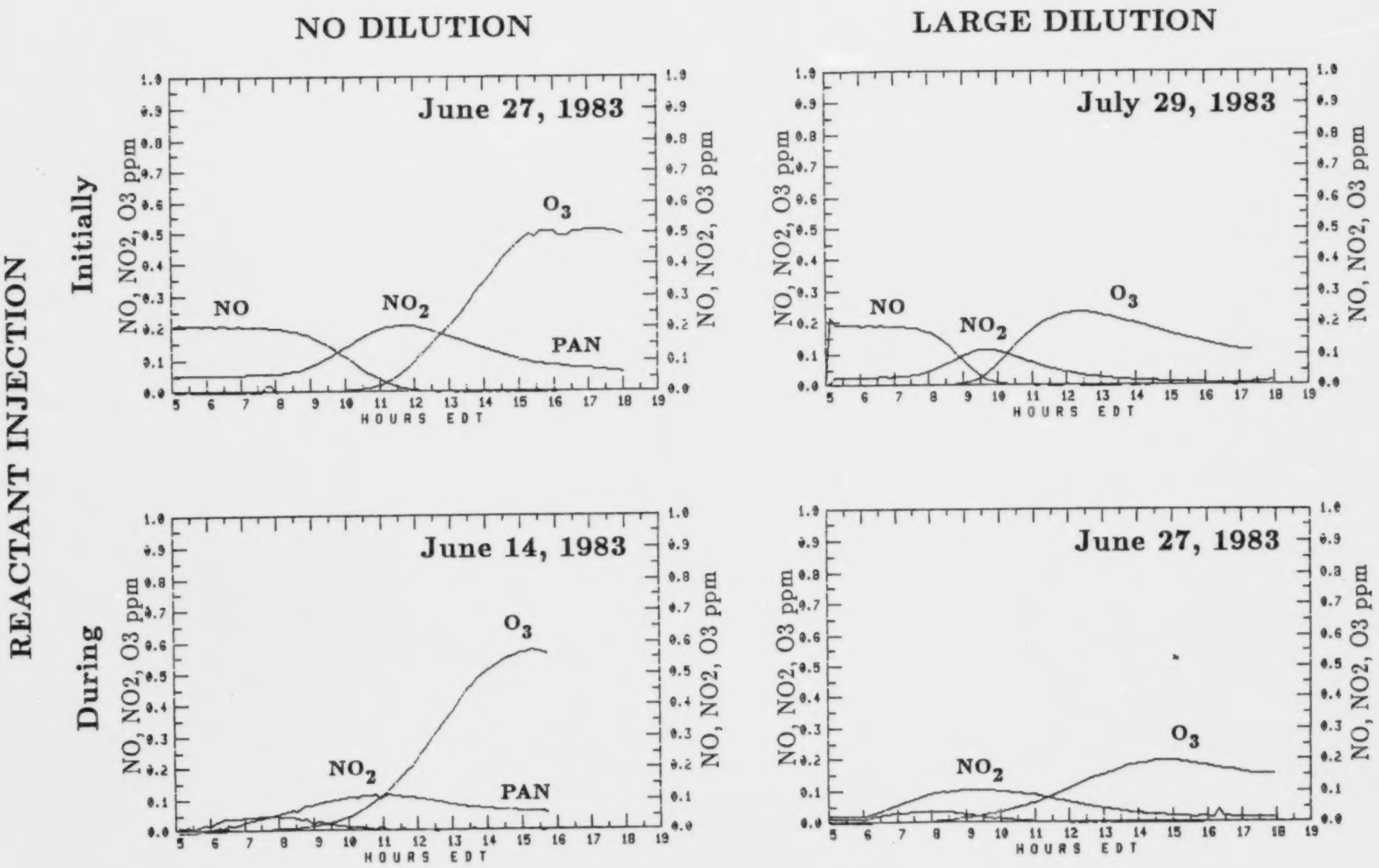

Figure 4. Outdoor smog chamber runs as examples of hierarchial experimental conditions. The NO_x concentration was ≈0.25 ppm, HC concentration ≈2.6 ppmC of propylene/n-butane/toluene mixture. Large dilution means that 20% of initial mass is left after 10 hours of dilution (equivalent to mixing height rise from 250 m to 1250 m).

- when mechanisms fail in the comparison, "debugging" experiments are needed to assist in understanding why they failed; these types of experiments remove some of the complexity of the urban-like simulation to make the cause and effect relation clearer;
- the Whitten strategy of "bottom up" construction and testing of complex mechanisms requires a series of conditions to avoid the ambiguity of offsetting errors and to increase the degree of understanding of the workings of the complex description being constructed.

Previous Work

Three other projects using the UNC Outdoor Smog Chamber have contributed data for model testing. Although these projects had their own goals and purposes, they were not designed or performed totally independently of each other or of this project. Instead, to the extent possible, each project depended upon data from other projects to address specific issues. Thus data from these projects are needed to complete the partial description provided by the specific work performed in this project. These other projects are briefly described below.

1977-81 Data Set

The predecessor to the present project produced 114 dual-experiments designed to test explicit mechanisms for aldehydes, olefins, paraffins, and simple two-component mixtures. These data were described in a final report[12] and a magnetic tape containing the data was sent to the National Technical Information Service[13] and to several EPA-sponsored model-development groups.

The final report described guidance for modeling the data including recommendations on treatment of light data, dilution rates, wall losses, and use of water vapor and temperature data. These guidelines are still applicable to the data described in this report.

Reactivity Data Set

Another 70 dual-experiments were produced as part of a 1981–83 EPA grant[14] that investigated how well models could represent reactivity changes in simple and complex HC mixtures. The best of these experiments also have been distributed to the model development groups at SAI and the University of California at Riverside (UCR).

Automobile Exhaust Data Set

Another 31 dual-experiments using automobile exhaust from two vehicles were produced as part of a 1982–84 EPA cooperative agreement. These experiments were described in detail in a final report,[15] and the processed data have also been sent to SAI and UCR for model testing.

Purpose

The purpose of this research project was to:

- measure reactant and product concentrations as functions of time in selected photochemical smog systems;
- process these data into a form readily distributable to model developers and testers; and
- provide auxiliary information needed to create mathematical model descriptions of the systems.

The types of systems investigated in this work included experiments to further test the aromatic portions of mechanisms, experiments to test representation of simple mixtures, and experiments to test mechanisms in dynamic situations. This project produced 128 dual-experiments.

These 128 experiments, when added to the other experiments in the whole database, encompass a range of complexity from single HC species in totally static situations to complex urban mixtures in fully dynamic conditions. These latter situations include time varying HC mixture compositions. The data set, as a whole, is well suited to develop and test models of chemical transformations in polluted atmospheres. These mechanisms can then be used with increased confidence in air quality simulation models (AQSMs), such as the EKMA model or the regional oxidant model, to provide control estimates for HC and NO_x needed to meet the standard for O_3.

The purpose of this report is to organize the 345 dual-experiments that are now part of the total database so that model developers can readily select experiments to test various aspects of their models. Because of the data density and complexity, the experimental data are usually supplied on magnetic tape or floppy disk in a format that includes extensive documentation with the data. The format allows reasonably simple computer programs to read the data into formats used by individual modelers for their own needs. The experiments usually appear in chronological order on the data tape.

The 345 dual-experiments described in this report include those performed in the three other projects and thus the data set includes data collected from 1977 through 1983. These other experiments complement and strengthen those performed in the three-year 1981–83 study reported here.

2

Organizing Principles

The 345 experiments from all four projects cover such a complex domain that multiple organizing principles are needed. These might be thought of as "keys" used to access a group of runs. Six kinds of attributes are used to organize the runs in the data set:

- ▹ class of run
- ▹ experimental conditions
- ▹ experimental series
- ▹ quality of run
- ▹ processing status of run
- ▹ project that produced the data

These are described below.

Class of Run

Two basic types of experiments are conducted in the chambers: characterization runs that address unique aspects of the UNC chamber performance and organic/NO_x runs to test mechanism design. Further, either of these type of experiments can occur on a single day or they can last one-and-a-half or two days. This organizing dimension is called the *Class* of the run. The classes of runs that are included in our database follow.

Chamber Characterization Class

These runs include experiments designed to provide chamber-specific data such as:

- How much O_3 is produced in a "blank" chamber filled only with background (clean, rural) air?
- What is the magnitude of NO_x emissions from the chamber walls?
- What is the rate of NO-to-NO_2 oxidation produced by the background air used to fill the chamber?
- What is the O_3 decay rate in the chamber?
- What is the photolysis rate of aldehydes?

In addition, multi-day characterization runs are needed to test overnight processes such as dark decay losses and wall emissions on subsequent days. More than 12% of the runs in the data set are in this class.

One-day, Organic/NOx System Class

These runs are mainly designed to test a chemical aspect of a mechanism such as:

- Can a mechanism that adequately describes the chemical transformations in a propylene-only system describe those in an ethylene/acetaldehyde system?
- Does a given mechanism work well over a range of dilution rates?
- Does a given mechanism work well over a range of HC-to-NO_x ratios?
- Does a given mechanism work well over a range of temperatures?
- Does a given mechanism work for two different compositions of a mixture of the same species?

About 85% of the runs in the data set are in this class.

Multi-day, Organic/NOx System Class

These runs are needed to test the relationships between the light and dark processes and to see if the products from the first day's reactions are adequately treated on the second day's irradiation. The present data set includes only a few runs in this class.

Experimental Conditions

Table 1 described a hierarchy of experimental conditions that can be used to organize experiments along a dimension of simple to complex, adding only one new factor at each level. The major characteristics used are: conditions for dilution and injection, type of HC system used, *i.e.* single HC species or mixture, and, if a mixture, whether the composition is constant or varying over time. These characteristics are of two types: physical and chemical.

Physical Conditions: Light, Dilution, Injection

This category describes the three principle physical operating conditions of chambers:

- type of irradiation: constant, artificial light or natural sunlight;
- magnitude of dilution: minimal dilution or large, atmospheric-like dilution;
- introduction of reactants: reactants added only at the start of a run or fresh reactants added throughout the experiment.

This scheme gives rise to eight basic types of runs.

Since the UNC chamber is an outdoor chamber, the four combinations using constant light intensity are not possible in our work. Other chambers such as the evacuable chamber at UCR or the Batelle chamber have to be used for these more simple conditions. Both of these facilities have supplied data to EPA-funded model developers.

In later discussion, experiments are classified by the two attributes Dilution and Injection into four basic kinds of runs. For those experiments in which reactants were injected throughout the run, additional sub-categories are used to indicate which reactants, HC, NO_x, or both were dynamically injected.

In each of the four basic types of runs created by the combinations of dilution and injection, a hierarchy of organic reactants can be developed. Other experimental attributes are therefore required to organize the database within the physical conditions.

Chemical Conditions: Number of Compounds, Composition

The simplest type of organic reactant run would be for a single organic species and

NO_x. Within the single species type of runs, the Whitten *Hierarchy of Species* can be applied. The complexity of the situation can be increased incrementally by moving from single species of each organic type to mixtures of organic types and then to multi-component mixtures. The latter situation introduces another category for mixtures involving composition.

An ultimate test of a mechanism designed for use in urban situations would be its ability to correctly predict the effects of a dynamic variation in the HC mixture composition throughout a run. That is, can the model predict the correct O_3 and NO_x transformations in a HC mixture in which the paraffin/olefin/aromatic ratio was changing throughout the run because the composition of the organics injected during the run was varied.

In later discussion, experiments are classified by a HC-type that indicates the types of organic reactants used. Other experimental attributes are the concentration and species identities for the reactants. The initial NO_x concentration and up to three initial concentrations and species or mixture identities are used to organize the experiments.

Experimental Series

All runs fit into the dimensions described above, *e.g.* a one-day, organic/NO_x system, normal dilution, reactants injected only before sunrise, simple mixture, constant composition run. Experiments were done, however, to test some specific aspect of the chemistry and often the results need to be compared with those from other similar experiments to obtain the full meaning of a particular experiment. To accommodate these relationships in the organization, we use the concept of an *Experimental Series*.

We have divided these series into three general categories: the first category, side-by-side series, are those series that describe the basic relationship between the chemical systems in the two chamber halves; the second category, chemical properties series, are those series that describe the chemical question being addressed in the experiment; the third category contains series for those runs that were used to characterize the chamber.

Side-by-Side Series

These series describe the relationship between the two sides of the chamber during an experiment. There are six basic kinds of relationships in these series:

- **Matched Conditions**—Both sides of the chamber have exactly the same chemical systems. The primary purpose for this type experiment is to show that the two chamber halves perform identically for the various chemical systems being tested. This allows stronger conclusions about cause-and-effect to be drawn in other experiments with different conditions in the two sides.
- **Relative Reactivity**—Conditions on the two sides of the chamber are matched except for organic reactant identity. Generally these experiments have the same NO_x concentrations and often have the same HC concentrations, except when the reactivity of the two hydrocarbons being studied is greatly different. This allows the relative behavior of one chemical system to be compared to that of another chemical system. Typically one chamber side has a reasonably well understood (*i.e.* readily modelable) system, and the other side has a system in which the chemistry is less well understood. Alternatively two systems, neither of which are well understood, can be compared.
- **Substitution**—Conditions on the two sides of the chamber are matched except that part of the carbon in the organic mixture is replaced with the same amount of carbon but with a different species identity. For example, one side of the chamber might contain 1.5 ppmC butane and 0.6 ppmC propylene for a total concentration of 2.1 ppmC; the other side might contain 1.0 ppmC butane, 0.4 ppmC propylene and 0.7 ppmC toluene for a total concentration of 2.1 ppmC. In this example, one-third of the butane/propylene mix was replaced with toluene. This differs from the Relative Reactivity type of experiment in that it is used only for mixtures and only about 25–33% of the carbon is substituted.
- **Addition**—Conditions on the two sides of the chamber are matched except that additional organic reactants are added to one side. The additional reactants could be a single compound such as CO or HCHO or it could be a mixture.
- **Delta Concentration**—The NO_x concentration and the organic reactant being studied are the same on the two sides of the chamber but the HC concentration is different. Conversely, the HC concentration and composition might be the same on the two chamber sides, but the NO_x concentration might be different. Since most control strategies are for HC reduction, most experiments of this type are ones in which the HC has been reduced while the NO_x remains the same on the two sides. These experiments validate the model's ability to predict $\Delta O_3/\Delta HC$ correctly with all other conditions being the same.
- **Static vs. Dynamic**—One side of the chamber has normal dilution (typically

less than 10%) with all reactants injected before sunrise; the other side of the chamber has the same set of reactants but the chamber is diluted to a large extent (typically by a factor of 5) or one or both of the reactants are injected into the chamber throughout the experiment with or without dilution. The chemical conditions are generally such that, if no reaction had taken place and no dilution had occurred, the chamber conditions would be matched after 10 hours.

Chemical Properties Series

These series include:

- **Hydrocarbon Class**—One side of the chamber has a single organic species and the other side has a different organic species: NO_x concentrations are the same on both sides. This type of series includes not only comparison of one species with another species in a given class but also comparison of a species in one HC class with a species in another HC class (*e.g.* comparison of the relative reactivity of propylene with toluene).
- **Mixture Representation**—A single species is compared with a simple mixture of two or more species; or a simple mixture is compared with a more complex mixture; or a mixture with one composition is compared with a mixture of the same species but a different composition.
- **Temperature, Light, and Humidity Effects**—Chemical systems run on one day are compared to similar chemical systems run on a different day with a different temperature profile, a different water vapor concentration or a different solar radiation profile.
- **Replicate experiments**—Chemical systems run on one day are compared to similar chemical systems run on a different but similar day. Matched propylene experiments are often in this series. For example, a propylene run conducted on August 13, 1981 might be compared to the identical experiment conducted on August 20, 1984.
- **Others**—Series that have few experiments or have unusual conditions. One example is an "All NO_2" series in which the initial NO_x was all NO_2.

Characterization Series

For the sake of clarity, characterization runs are placed in their own set of series. These include:

- **Background Air only**—Effectively a "blank" run. No reactants are injected, the chamber is simply closed and monitored.
- **NO oxidation, Background Air**—NO is injected into chamber background air and the oxidation rate is monitored on both sides of chamber.
- **NO oxidation, CO added**—NO is injected into chamber background air; 50 to 100 ppm of CO is added to one side of the chamber to serve as a simple, radical-oxidizable species. This usually enhances the NO oxidation rate.
- **Aldehyde added**—Similar to a "Background-Air only" test, but an aldehyde, usually acetaldehyde, is added to one side of the chamber to serve not only as a large radical source, but also, in the case of acetaldehyde, to convert any NO_x emitted from the chamber walls to PAN. The amount of O_3 and PAN formed can indicate the extent of NO_x emissions from the chamber walls.
- **Decay of Species**—Similar to a "Background-Air Only" test, but various species such as O_3, HNO_3, or other reactive species are injected to determine the loss rate to the walls for these species.

Runs in Multiple Series

The 345 runs are first classified into one of the 15 side-by-side series or one of the 6 characterization series. These will be described in detail in a later discussion. In addition, a run may also appear in one or two of the 19 chemical properties series. Many runs appear in more than one series, for example, a relative reactivity run will also be a simple to complex mixture transition run and also be a replicate experiment. This situation actually forms a network of runs allowing for various cross-checking in tests. For purposes of this report, we have arbitrarily limited the number of experimental series that a given run might be included in to three.

Within an experimental series a run has a *rank*. The exact meaning of the rank may vary depending upon the nature of the series, but usually it would indicate the relative order of complexity of the run in the series or the probable order that the run should be simulated in when testing mechanisms.

Quality of Run

Experiments are rated on a scale of 0 to 9 (highest). The major determining factors in the quality are the weather conditions, especially the sky cover, direct sunlight, and haze conditions, and the number and performance of the analytical instruments, especially those used for product data. Grading techniques will be discussed later.

Processing Status of a Run

Not all experiments are processed. Runs are assigned a priority for processing based upon the experimental conditions, the number of instruments that produced data, and the extent to which the run conditions provided unique information. Some runs have such poor sunlight or weather that they are not suitable for model testing purposes. Others have instrument problems that significantly lessen the utility of the run to test choices in the mechanism construction. Still others are judged to have a lower priority relative to other runs and they are not fully processed within the time and funds provided on the project. These remain in a semi-processed state.

Some modelers have expressed interest in *all* runs performed, whether fully processed or not. In part, this is to provide insight into any potential run-to-run contamination effects and in part, because the modeler may need information from a run we have not processed yet. To meet these needs, *all* runs performed since 1981 are included in the data base and a processing status is used to indicate the availability of the data on tape or other form. Only runs that were fully processed in the 1977 to 1980 data set are included; no entries were made for partial or unprocessed runs from this period. This information can be supplied, however, in paper-form on special request.

Project That Produced The Data

All runs are assigned a project name to identify the project that produced the experiment. Thus all automobile exhaust runs can be found by searching for runs with a project name of AUTO.

Summary of Organization

Table 3 summarizes the categories and run characteristics that have been described above. These terms and symbols will be used throughout the remainder of the report when discussing runs.

Experimental Conditions Database

To aid modelers in searching for test conditions, the entire Experimental Conditions Database is available on various magnetic media. This database uses codes, similar to those in the summary table (Table 3), to compress the information into a reasonably small form. Although it is expected that most users will place the database on a computer and use a database query language capable of easily translating the codes into english for reports, the database is not that difficult to search by hand. For this reason, and to aid programmers in loading the database on their computers, we have included the entire database in printed form in Appendix A. Each line of the listing in Appendix A represents one run and is about 100 characters long. The appendix also includes a full description of the record format and gives translations for all the coded fields in the record.

Table 3. Summary of Run Organization

Run Date	The primary identifying key for experiment.
Class	One of the following types ▷ C —Characterization experiment; ▷ D —Characterization experiment, second day; ▷ O —One day organic NO_x experiment; ▷ T —Two day organic NO_x experiment, first day; ▷ S —Two day organic NO_x experiment, second day.
Dilution	One of the following types ▷ N —Normal dilution (ca. 10%/day); ▷ D —Large dilution (ca. 5-fold dilution in 10 hours);
Injection	One of the following types ▷ I —All reactants injected, before sunrise; ▷ H —HC injected during experiment, NO_x injected before sunrise; ▷ N —NO_x injected during experiment, HC injected before sunrise; ▷ B —Both HC and NO_x injected during experiment; ▷ C —Combination injection different from above.

Table 3. Summary of Run Organization, cont.

`HC Type` First letter designates one of the following types

`1` Single species on each side of the chamber. The letter following "`1`" designates the HC class of species as follows:

- ▷ `A` —aldehyde on each side;
- ▷ `O` —olefin on each side;
- ▷ `P` —paraffin on each side;
- ▷ `R` —aromatic on each side;
- ▷ `U` —olefin one side, aldehyde other side;
- ▷ `V` —olefin one side, paraffin other side;
- ▷ `W` —olefin one side, aromatic other side;
- ▷ `X` —some other combination.

`M` Mixture on at least one side of the chamber. The letter following "`M`" designates the mixture complexity as follows:

- ▷ `B` —simple mixture of two or three species;
- ▷ `C` —named mixture or mixture of named mixtures;
- ▷ `V` —mixture with time varying composition.

`Initial Conditions`

Gives the initial NO_x and HC concentrations and HC species identifications on the two sides of the chamber. Up to three individual HC species or mixtures are given for each side.

Table 3. Summary of Run Organization, cont.

Project A four letter code for the project as follows:

- ETPM—The present project or if before 1981, the previous project;
- REAC—The reactivity grant project, primarily dealing with mixtures and mixture compositional changes;
- AUTO—The automobile exhaust smog chamber project, dealing with the relative reactivity of exhaust from two vehicle, with two gasolines;
- AURE—Combination experiments performed for both the AUTO and the REAC projects.

Quality A grade from 0 to 9 (highest) for the experiment based largely on the sunlight, but also including instrument performance, product data availability, and need.

Processing Status

A one letter indicator of the processing status of the run, as follows:

- S —A fully processed and documented run, available for distribution on magnetic media.
- P —A partially processed run, currently being processed, available in graphical form with estimated initial conditions of ca. ±20%.
- L —A partially processed run of low priority, available in graphical form for raw data with target initial conditions of ca. ±20% for NO_x and initial HCs. This type run may never be fully processed.
- N —Not to be processed, not available.
- U —Unprocessed run; a processible run but no processing has occurred.
- —(blank state), status unknown.

Table 3. Summary of Run Organization, cont.

`Number`	The number of instruments used to take HC data for the run. Pre-1981 runs currently do not have this information and for these a 0 is used. Each HC instrument can measure several species so this number is only a general indicator of the amount of information available.
`Series1`	The experimental series that describes the side-to-side conditions of the run. These are ▷ `Matched` —Both sides identical; ▷ `Relative Reactivity` —Species identities different; ▷ `Substitution` —Carbon replaced by different species; ▷ `Addition` —Additional carbon added to one side; ▷ `Delta Conc.` —Different absolute HC or NO_x on sides; ▷ `Dynamic` —Conditions change through out run.
`Series2,3`	The experimental series that describe the chemical tests conducted. These include ▷ `HC Class` —Comparison of different HC within and across classes; ▷ `Mixture Representation` —Comparison of different mixtures and their composition; ▷ `Physical Conditions` —Comparison of temperature, water vapor, light intensity effects; ▷ `Replicate Experiments` —Essentially duplicate experiments on different days and years.
`RANK1,2,3`	Relative position of run in series.

3

Overview of Data Set

The purpose of this chapter is to provide a general view of the data set and to present information on how runs were classified.

Period Covered, Distribution

Table 4 gives the yearly distribution of experiments. Those from 1977–80 were included in the previous report.[12] The number of runs listed for these years only include those experiments that have been fully processed. Three different projects were producing data in 1982.

Table 4. Distribution of Experiments by Year

Year	Runs
'77	18
'78	45
'79	28
'80	23
'81	67
'82	90
'83	74

Table 5 gives the distribution of runs by project.

Table 5. Distribution of Experiments by Project

Project	Runs
Exp. Test Photo. Mech. 1978–80	114
Exp. Test Photo. Mech. 1981–83	128
HC Reactivity	72
Automobile Exhaust	31

Table 6 shows that experiments were performed mainly in the summer months, especially in July and August; a few experiments were performed in every month, however, to provide data on temperature and solar effects.

Table 6. Distribution of Experiments by Month

Month	Runs
Jan	3
Feb	1
Mar	2
Apr	1
May	4
Jun	55
Jul	70
Aug	74
Sep	59
Oct	50
Nov	23
Dec	3

The number of runs in each *Class* is given in Table 7.

Table 7. Distribution of Experiments by Class

Class	Runs
Characterization	34
Second day, Char.	12
One day, regular	293
Two day, regular	3
Second day, reg.	3

The breakdown of the runs by dilution and injection conditions is shown in Table 8.

Table 8. Distribution of Experiments by Dilution and Injection Conditions
(codes in () are defined in Table 3, page 27)

Dilution	Injection	Runs	Total
Large (D)			
	Continuous (B)	3	
	Initial (I)	2	
			5
Normal (N)			
	HC Continuous (H)	5	
	HC & NO_x Continuous (B)	7	
	HC Composition Varying (H,MV)	1	
	Initial Only (I)	327	
			340

Compounds and Mixtures Used

Table 9 gives a summary of experiments by the HC type. "Single" means that a single species was used on each side of the chamber. The second part of the code indicates the HC class of the two species. A "simple mixture" has two or three species. A "complex mixture" has at least four species and can have several hundred (*e.g.* exhaust). The complex mixtures used in the UNC experiments have been assigned names. The names and compositions of these complex mixtures are given in Table 10 and Table 11. An MC-type of experiment can also include a blending of two or three of the mixtures appearing in Tables 10 and 11.

Table 9. Distribution of Experiments by HC Type
(codes are defined in Table 3, page 29)

Code	HC Type	Runs
1A	Single, aldehydes	34
1O	Single, olefins	86
1P	Single, paraffins	11
1R	Single, aromatics	7
1U	Single, ole vs ald	15
1V	Single, ole vs par	2
1W	Single, ole vs aro	3
1X	Single, other	7
	Sub-total	164
MB	Mixture, simple	36
MC	Mixture, complex	97
MV	Mixture, varying	3
	Sub-total	135
B	Background air	41

Table 12 lists all the species and the mixtures used in all the experiments. The number given in the table is the number of chamber sides in which the species or mixture appeared. Note that this table only includes cases in which the species or

Table 10. Composition of Hydrocarbon Mixtures used in UNC Smog Chamber Experiments.

Compound	SIMMIX1	SIMMIX2	UNCMIX	SIMARO	COMARO	AUTO-0	AUTO-1A	AUTO-1B	P/B	P/B/T	BASMIX
butane	0.4002	0.4539					0.0391	0.0391	0.7663	0.5352	0.3140
pentane	0.3183	0.3610	0.2531							0.1268	
isopentane			0.1484			0.0550	0.0519	0.0519			
2-methylpentane			0.0996								
2,4-dimethylpentane			0.0864								
2,2,4-trimethylpentane			0.1202				0.1121	0.1121			
ethylene	0.1631	0.1850	0.1167			0.4000	0.2391	0.2391			0.0650
propylene	0.1184		0.0524			0.2200	0.0416	0.0416	0.2337	0.1648	0.0943
1-butene			0.0254				0.0196	0.0196			
trans-2-butene							0.0196	0.0196			
cis-2-butene			0.0313								
2-methyl-1-butene			0.0347								
2-methyl-2-butene			0.0317								
benzene							0.0538	0.0538			
toluene				0.4886	0.2482	0.2000	0.2115	0.2115		0.3000	0.2000
m-xylene				0.3860	0.1882					0.2000	
o-xylene							0.0481	0.0481			
1,2,4-trimethylbenzene				0.1234	0.2803	0.1250	0.0564	0.0564			
n-propylbenzene					0.1371						
sec-butylbenzene					0.1522						
formaldehyde							0.0200	0.0200			
acetaldehyde											
CO								AUTO[1]			
total paraffin	0.7185	0.8150	0.7077	0.0000	0.0000	0.0550	0.2031	0.2031	0.7663	0.5352	0.4408
total olefin	0.2815	0.1850	0.2922	0.0000	0.0000	0.6200	0.3199	0.3199	0.2337	0.1648	0.1593
total aromatic	0.0000	0.0000	0.0000	1.0000	1.0000	0.3250	0.4724	0.4724	0.0000	0.3000	0.4000

[1] $[CO]_{synthetic}$ matched to $[CO]_{vehicle}$

Table 11. Composition of Hydrocarbon Mixtures used in UNC Smog Chamber Experiments.

Compound	TOL-XYL-MIX1	TOL-XYL-MIX2	TOL-XYL-MIX3	TOL-TMB-XYLS	ISO-/2,2,4-TM-PENTANES	DODGEMIX II
butane						0.6449
pentane						
isopentane					0.5000	
2-methylpentane						
2,4-dimethylpentane						
2,2,4-trimethylpentane					0.5000	
ethylene						0.0615
propylene						0.0810
1-butene						
trans-2-butene						0.0498
cis-2-butene						
2-methyl-1-butene						
2-methyl-2-butene						
toluene	0.5000	0.6666	0.6666	0.4213		
m-xylene	0.5000	0.3334	0.1667	0.2572		
o-xylene			0.1667	0.1984		
1,2,4-trimethylbenzene				0.1231		
n-propylbenzene						
sec-butylbenzene						
formaldehyde						0.0146
acetaldehyde						0.0098
CO						
total paraffin	0.0000	0.0000	0.0000	0.0000	1.0000	0.6449
total olefin	0.0000	0.0000	0.0000	0.0000	0.0000	0.1953
total aromatic	1.0000	1.0000	1.0000	1.0000	0.0000	0.1385

Table 12. Number of Chamber Sides Containing Species

Species	Sides
BACKGROUND	46
CO	26
FORMALDEHYDE	31
ACETALDEHYDE	53
PROPIONALDEHYDE	2
ETHYLENE	43
PROPYLENE	178
1-BUTENE	8
TRANS-2-BUTENE	6
ISOPRENE	22
A-PINENE	9
METHACROLEIN	4
METHYLVINYLKETONE	4
METHYL ETHYL KETONE	5

Species	Sides
N-BUTANE	36
ISOPENTANE	1
N-PENTANE	1
2,3-DIMETHYLBUTANE	3
2,2,4-TRIMETHYLPENTANE	1
ACETONE	3
N-PROPYLNITRATE	1
N-BUTYLNITRATE	4
3-PENTANONE	4
ACETONITRILE	1
METHANOL	1

Table 12. Number of Chamber Sides Containing Species, cont.

Species	Sides
TOLUENE	43
ETHYLBENZENE	3
N-PROPYLBENZENE	5
M-ETHYLTOLUENE	1
M-XYLENE	18
O-XYLENE	13
1,2,4-TRIMETHYLBENZENE	4
BENZALDEHYDE	3
BIACETYL	7
METHYLGLYOXAL	8
GLYCOALDEHYDE	1

Mixtures	Sides
PRO/BUT MIX	15
DODGEMIX II	4
SIMMIX1	9
SIMMIX2	18
UNCMIX	93
COMARO	11
SIMARO	24
TOL/XYL/MIX1	6
TOL/XYL/MIX2	2
TOL/XYL/MIX3	2
TOL/TMB/XYLS	2
ISO-/2,2,4-TM-PENTANES	4
'72 DODGE AUTO EXHAUST DIRECT	31
'72 DODGE AUTO EXHAUST CRYO	7
'79 VOLARE AUTO EXHAUST DIRECT	18
SYNTHETIC AUTO EXHAUST 0	2
SYNTHETIC AUTO EXHAUST 1A	3
SYNTHETIC AUTO EXHAUST 1B	2

mixture was present by itself or with at most two other species or mixtures from Tables 10 and 11.

Experimental Series

Table 13 gives the number of runs in each of the side-by-side series or in each of the characterization series. The second day of regular runs are not included in the table.

Table 13. Distribution of Experiments by Series1.
(codes are from Appendix A Tables)

Code	Name	Runs	Total
007	Matched propylene	33	
008	Matched mixture	10	
009	Matched other	21	
			64
018	Reactivity Comparison	135	
			135
023	Substitution, UNCMIX	8	
024	Substitution, P/B	5	
025	Substitution, SIMMIX	2	
026	Substitution, Other	5	
			20
027	Addition, one species	3	
028	Addition, CO	5	
029	Addition, Ald	4	
030	Addition, Other	4	
			16
033	Delta HC	37	
034	Delta NOx	5	
			42
035	Static to dynamic	18	
			18
			295

Table 13. Distribution of Experiments by Series, cont.

Code	Name	Runs
001	Char; Background	9
002	Char; NO oxid. NO only	7
003	Char; NO oxid. CO added	9
004	Char; O3 decay	9
005	Char; NO2/O3, dark	4
006	Char; Ald. added	8
		46

Grading, Ranking

Quality Grading

A grading procedure is used to judge the quality of an experiment; it is done independently for each experiment. The grade is one factor in selecting experiments from the large dataset. Grades ranges from 0 to 9 with 9 being the highest quality. Although the assessment of the quality index is somewhat subjective, many characteristics can at least be placed in order on a relative scale.

The grade is calculated using a series of formulas and forms during data processing. There are five items that are graded individually from 0 to 9 and the total run grade is computed by averaging these five grades. The items that are graded are:

- Sunlight
- Initial Conditions
- Analytical Support
- Chamber Conditions
- Need/Usefulness

Sunlight

For the years 1977-80 the sunlight quality was the principle factor used to represent run quality. The grade was assigned by comparing the solar radiation profile with a series of graded TSR profiles and the grade of the profile that most closely fit was assigned to the run. The graded profile set was published in the previous project final report.[17]

In 1981 a formula was developed which grades the sunlight quality more quantitatively but is still consistent with the general technique used earlier. This formula uses the percent of possible solar radiation received for the day, the number times clouds blocked direct sunlight (called "holes or dips" in the profile), and the occurance of morning fog or haze to calculate a grade.

The morning sunlight is more important in modeling the runs than the afternoon sunlight and, therefore, the first half of the day is weighted 70% in generation of the sunlight quality grade. Meteorological data obtained at a major airport (RDU), about 50 km from the site, lists percent of possible sunshine data. This data correlates well with the chamber site observed TSR profiles. This value is used to establish the starting grade value: 90–100 percent is converted to a quality grade of "9" and so-forth. The TSR profile from the experiment is examined for local clouds that cause "holes" in the profile. Clouds resulting in 25% or more attenuation are counted into three classes: 15, 30 and 60 minute duration. Points are subtracted for each "hole" weighted by duration class.

Initial Conditions

Three items contribute to this grade: degree of achieving desired target conditions for total NO_x and HC, degree of achieving desired ratios of reactants in each side and between the two chamber sides, and degree to which the experimental conditions were quantifiable or verifiable.

The initial grade is set to "9". One grade point is deducted for each 20% deviation from the absolute target condition. For the dual chambers, it is the relative ratios of the initial reactant concentrations that are more important than the absolute concentrations. If a mixture is used, the relative fractions of components need to be established. Two types of relative comparisons are made: the ratios of components to each other within a mixture and the ratios of components in two different mixtures (side by side comparison). Sometimes the initial condition of interest is a matched HC to NO_x ratio. One grade point is deleted for each 5% deviation from the target ratio.

Usually initial conditions are verifiable analytically. When an analytical techniques fails or a sample is not taken before the beginning of an experiment, other techniques may have to be used to establish or estimate the initial conditions. Direct injection of neat liquids or gases are often used as a calibration technique and therefore can be used as a second-best estimate of initial conditions. If a component of a commonly used mixture is not directly analytically monitored for a particular experiment, its concentration can be estimated from the concentrations of the other mixture components and relative composition data. However these techniques are less than ideal and two grade points are deleted from this quality category for each initial compound not verified by an analytical technique.

Analytical Support

Analytical support is not always available for all species for all runs: instruments sometimes fail during an experiment. The base grade is set at "9" and grade points are deducted, weighted by importance of the species or physical data not measured.

Chamber Conditions

Chamber conditions can have a major impact on experimental results. Important parameters include: condensation on walls, dilution rate, and hours of venting before the experiment. The initial grade for this item is set at "9".

Condensation observed on chamber walls is noted by the operator starting the experiment. One grade point is deducted if condensation is observed in both chambers. Chamber driers do not always operate well and sometimes one side may be dried better than the other resulting in condensation in one side only. Two grade points are deducted for this situation.

Dilution rate is usually monitored by use of inert tracers such as CCl_4. An exponential, least-squares analysis of this tracer data is used to determine the dilution rate (necessary for proper modeling) for each chamber. Dilution rates are normally well matched and less than 1% per hour.

One point is deducted from the grade if the dilution rates on the two sides differ by more than 20%. Additional points are deducted for dilution rates exceeding the normal dilution rate of 1.5×10^{-1} min^{-4}. Two points are deducted if the dilution rate is not quantifiable because of incomplete or poor tracer data. One point is deducted if the dilution rate is high or irregular because of windy conditions.

Two hours of venting will eliminate observable concentrations of chamber pollutants. Regular experimental protocol requires that each run be preceded by at least six hours of venting. Three grade points are deleted if less venting time is used.

Need/Usefulness

An important aspect of an experiment is its overall usefulness and value. Many experiments are conducted to satisfy questions requiring immediate attention or special effort. Often these experiments are difficult to conduct; the experimental quality may be less than desired but nevertheless the experiment contributes useful information which may be unavailable otherwise. These experiments may be supportive of other experiments. This category is used to adjust the quality grade to reflect these experimental needs. It can change the final run grade by at most one.

Distribution of Runs by Quality

Table 14 shows the distribution of runs by Quality.

Table 14. Distribution of Experiments by Quality

Quality	Runs
9	62
8	89
7	85
6	30
5	43
4	18
3	8
2	7
1	2
0	1

Series Ranking

The purpose of ranking runs in a series is to aid in selecting runs from the database for model testing. Two ranking procedures are used depending upon the series: the first ranking, into five broad categories, is applied to the side-by-side series;

the second ranking, the recommended order of simulation, is applied to special test series or species hierarchy series.

In the side-by-side series, the runs are further sub-divided by the hydrocarbon type used in the experiment. Within the HC type, runs are ranked into the broad categories described in Table 15.

Table 15. General Run Rankings

Category	Rank Range
Best in HC type	1
Best of kind	2–10
Satisfactory	11–50
Supporting	51–100
Some Problems	101—500
Not for modeling	999

For example, there may have been two runs that demonstrated the relative reactivity of iso-pentane and n-butane at two different HC concentrations. If these runs were judged to be modelable, both of these runs would be ranked in the "Best of kind" range because they were the only ones we had of this type. This means each run has a numerical rank between 2 and 10. One run might be 5 and the other 10 because the weather conditions might have been better for the former.

Several "Best of kind" might also appear within a single HC type within a given series because different species were used. The category "Best of HC type" would be used to select the best run of the "Best of kind" within the HC type. The database may not have a "Best of HC type" because none of the "Best of kind" experiments were considered good enough for that designation.

4

Runs by Series

The purpose of this chapter is to group the 345 experiments into seven lists based on the principle series into which each experiment falls. The lists are presented in Tables 16–22. The seven experimental series are: characterization (Table 16), matched (Table 17), relative reactivity (Table 18), substitution (Table 19), addition (Table 20), delta concentration (Table 21), and static to dynamic (Table 22).

Within each series list, the runs are grouped by HC type beginning with the simplest type that appears in the series. Within the HC type grouping, the runs are in chronological order.

The first three letters following the run date in these tables are the codes for the Class, Dilution, and Injection conditions (as defined in Table 3). The initial conditions for NO_x and up to three HC reactants or HC mixtures are listed next. The four letter codes listed for "Proj" denote the project under which the data were obtained. The next three codes represent the run quality, number of HC instruments used and the current processing status as defined in Table 3. Finally, guidance for the usefulness of a specific run is given in terms of the general ranking categories as defined in Table 15.

Characterization Runs

Table 16.

********** For the Series Char;Background Air Only **********

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
11-Aug-78 CNI	0.005		BACKGROUND	ETPM	5	0	S	Satisfactory
	0.004		BACKGROUND					
15-Jun-81 CNI	0.002		BACKGROUND	ETPM	7	6	L	Best of kind
	0.002		BACKGROUND					
16-Jun-81 DNI	0.000		TWO DAY CON'T	ETPM	7	0	L	Best of kind
	0.000		TWO DAY CON'T					
17-Jun-81 CNI	0.002		BACKGROUND	ETPM	7	6	L	Best of kind
	0.002		BACKGROUND					
18-Jun-81 DNI	0.000		TWO DAY CON'T	ETPM	7	0	L	Best of kind
	0.000		TWO DAY CON'T					
6-Jun-82 CNI	0.004		BACKGROUND	ETPM	8	5	S	Best of kind
	0.012		BACKGROUND					
7-Jun-82 DNI	0.000	1.00	ACETALDEHYDE TWO DAY CON'T	ETPM	8	0	S	Supporting
	0.000	1.00	ACETALDEHYDE TWO DAY CON'T					
16-Jun-82 CNI	0.000		BACKGROUND	ETPM	8	4	S	Best of kind
	0.000		BACKGROUND					
21-Sep-83 CNI	0.000		BACKGROUND	ETPM	7	5	P	Satisfactory
	0.000		BACKGROUND					

Number of runs for this Series is 9

Table 16. Characterization Runs, cont.

********** For the Series Char;Background Air **********

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
2-Aug-81 CNI	0.500		BACKGROUND	ETPM	7	4	U	Not for model
	0.500		BACKGROUND					
17-Sep-81 CNI	0.362		BACKGROUND	ETPM	9	4	S	Best of kind
	0.363		BACKGROUND					
18-Sep-81 DNI	0.362		BACKGROUND TWO DAY CON'T	ETPM	9	0	S	Best of kind
	0.363		BACKGROUND TWO DAY CON'T					
17-Jun-82 DNI	0.500		TWO DAY CON'T	ETPM	8	0	S	Satisfactory
	0.500		TWO DAY CON'T					
8-Oct-82 CNI	0.304		BACKGROUND	ETPM	7	4	S	Satisfactory
	0.300		BACKGROUND					
24-Jul-83 CNI	0.309		BACKGROUND	ETPM	7	2	P	Satisfactory
	0.486		BACKGROUND					
11-Nov-83 CNI	0.600		BACKGROUND	ETPM	8	3	U	Satisfactory
	0.600		BACKGROUND					

Number of runs for this Series is 7

Table 16. Characterization Runs, cont.

********** For the Series Char;NO oxid. CO added **********

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
14-Aug-78	CNI	0.522		BACKGROUND	ETPM	6	0	S	Best of kind
		0.523		BACKGROUND					
			49.20	CO					
27-Jun-82	CNI	0.456		BACKGROUND	ETPM	8	4	S	Satisfactory
			54.80	CO					
		0.446		BACKGROUND					
2-Aug-82	CNI	0.389		BACKGROUND	ETPM	8	4	S	Satisfactory
		0.388		BACKGROUND					
			45.40	CO					
20-Aug-82	CNI	0.411		BACKGROUND	ETPM	9	4	S	Best of HC type
		0.413		BACKGROUND					
			50.70	CO					
22-Aug-82	CNI	0.459		BACKGROUND	ETPM	8	4	S	Satisfactory
		0.457		BACKGROUND					
			40.40	CO					

Table 16. Characterization Runs, cont.

********** For the Series   Char;NO oxid. CO added   **********

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
23-Aug-82 CNI	0.437		BACKGROUND	ETPM	7	4	S	Satisfactory
	0.433		BACKGROUND					
		46.50	CO					
5-Sep-82 CNI	0.497		BACKGROUND	ETPM	8	3	S	Satisfactory
	0.492		BACKGROUND					
		50.00	CO					
27-Jul-83 CNI	0.464		BACKGROUND	ETPM	6	3	P	Best of kind
		48.60	CO					
	0.431		BACKGROUND					
6-Aug-83 CNI	0.333		BACKGROUND	ETPM	5	3	P	Satisfactory
		50.00	CO					
	0.331		BACKGROUND					

Number of runs for this Series is 9

Table 16. Characterization Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
********** For the Series			Char;03 decay			**********		
3-Jul-82 CNI	0.008		BACKGROUND	ETPM	8	5	S	Best of HC type
		0.45	03					
	0.008		BACKGROUND					
		0.50	03					
4-Jul-82 DNI	0.000		TWO DAY CON'T	ETPM	8	0	S	Best of HC type
	0.000		TWO DAY CON'T					
20-Oct-82 CNI	0.000		BACKGROUND	ETPM	3	3	L	Some problems
		0.56	03					
	0.000		BACKGROUND					
		0.53	03					
21-Oct-82 DNI	0.000		TWO DAY CON'T	ETPM	3	0	L	Some problems
	0.000		TWO DAY CON'T					
14-Aug-83 CNI	0.000		BACKGROUND	ETPM	9	4	S	Best of kind
	0.000		BACKGROUND					
15-Aug-83 DNI	0.000		TWO DAY CON'T	ETPM	9	4	S	Best of kind
	0.000		TWO DAY CON'T					

Table 16. Characterization Runs, cont.

```
   RUN
   DATE            NOx    HC                          Proj Q I P     GUIDE

********** For the Series   Char;O3 decay               **********

 24-Aug-83 CNI    0.000                               ETPM 5 2 P Satisfactory
                  0.000

 24-Oct-83 CNI    0.000          BACKGROUND           ETPM 8 3 P Satisfactory
                  0.000          BACKGROUND

 25-Oct-83 DNI    0.000          TWO DAY CON'T        ETPM 8 3 P Satisfactory
                  0.000          TWO DAY CON'T

Number of runs for this Series is     9
```

Table 16. Characterization Runs, cont.

********** For the Series Char;NO2/O3, dark **********

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
3-Aug-81 CNI	0.500		BACKGROUND	ETPM	4	4	L	Best of kind
	0.500		BACKGROUND					
4-Aug-81 DNI	0.000		TWO DAY CON'T	ETPM	4	0	L	Best of kind
	0.000		TWO DAY CON'T					
15-Nov-81 CNI	0.333		BACKGROUND	ETPM	8	4	S	Best of kind
	0.310		BACKGROUND					
16-Nov-81 DNI	0.000		TWO DAY CON'T	ETPM	8	0	S	Best of kind
	0.000		TWO DAY CON'T					

Number of runs for this Series is 4

Table 16. Characterization Runs, cont.

********** For the Series Char;Ald. added **********

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
21-May-79 CNI	0.004	2.81	ACETALDEHYDE	ETPM	7	0	S	Satisfactory
	0.004	0.83	ACETALDEHYDE					
21-Jul-79 CNI	0.009	2.00	ACETALDEHYDE	ETPM	4	0	S	Satisfactory
	0.015	2.00	ACETALDEHYDE					
17-Jul-82 CNI	0.003	0.52	FORMALDEHYDE	ETPM	8	5	S	Best of kind
	0.007	0.58	FORMALDEHYDE					
18-Jul-82 DNI	0.500		TWO DAY CON'T	ETPM	8	0	S	Best of kind
	0.500		TWO DAY CON'T					
13-Jul-83 CNI	0.000	1.00	ACETALDEHYDE	ETPM	5	5	L	Best of kind
		0.50	CO					
	0.000	1.00	ACETALDEHYDE					
26-Jul-83 CNI	0.020	0.97	ACETALDEHYDE	ETPM	8	5	S	Satisfactory
		54.90	CO					
	0.010	1.00	ACETALDEHYDE					
4-Aug-83 CNI	0.000		ACETALDEHYDE	ETPM	8	6	S	Satisfactory
		50.00	CO					
	0.000		ACETALDEHYDE					
25-Aug-83 CNI	0.000	1.00	ACETALDEHYDE	ETPM	8	6	P	Satisfactory
		50.00	CO					
	0.000	1.00	ACETALDEHYDE					

Number of runs for this Series is 8

Total number of runs is 46

Matched Runs

Table 17.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
********** For the Series Matched propylene **********								
8-Aug-77 ONI	0.499	1.54	PROPYLENE	ETPM	5	0	S	Best of kind
	0.501	1.50	PROPYLENE					
21-Oct-78 ONI	0.497	3.50	PROPYLENE	ETPM	9	0	S	Best of kind
	0.495	3.54	PROPYLENE					
22-Oct-78 ONI	0.490	1.40	PROPYLENE	ETPM	9	0	S	Best of kind
	0.487	1.40	PROPYLENE					
1-Jun-79 ONI	0.535	1.52	PROPYLENE	ETPM	5	0	S	Supporting
	0.537	1.52	PROPYLENE					
29-Jun-79 ONI	0.459	3.83	PROPYLENE	ETPM	6	0	S	Supporting
	0.452	3.78	PROPYLENE					
14-Oct-79 ONI	0.503	2.92	PROPYLENE	ETPM	9	0	S	Best of kind
	0.502	2.94	PROPYLENE					
24-Oct-79 ONI	0.456	3.55	PROPYLENE	ETPM	8	0	S	Satisfactory
	0.446	3.54	PROPYLENE					
2-Oct-81 ONI	0.500	4.00	PROPYLENE	ETPM	7	6	L	Satisfactory
	0.500	4.00	PROPYLENE					
18-Oct-81 ONI	0.500	4.00	PROPYLENE	ETPM	5	3	N	Supporting
	0.500	4.00	PROPYLENE					

Table 17. Matched Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
********** For the Series		Matched propylene		**********				
26-Oct-81 ONI	0.500	4.00	PROPYLENE	ETPM	0	3	N	Some problems
	0.500	4.00	PROPYLENE					
13-Apr-82 ONI	0.400	4.00	PROPYLENE	ETPM	2	2	N	Not for model
	0.400	4.00	PROPYLENE					
28-May-82 ONI	0.500	4.00	PROPYLENE	ETPM	2	4	N	Some problems
	0.500	4.00	PROPYLENE					
21-Jun-82 ONI	0.320	4.00	PROPYLENE	ETPM	5	6	L	Supporting
		3.00	CO					
	0.320	4.00	PROPYLENE					
		3.00	CO					
2-Jul-82 ONI	0.500	3.00	PROPYLENE	ETPM	8	4	L	Satisfactory
	0.500	3.00	PROPYLENE					
15-Aug-82 ONI	0.500	3.00	PROPYLENE	ETPM	7	3	U	Some problems
	0.500	3.00	PROPYLENE					
17-Aug-82 ONI	0.300	3.00	PROPYLENE	ETPM	3	3	U	Supporting
	0.300	3.00	PROPYLENE					
25-Aug-82 ONI	0.500	1.50	PROPYLENE	ETPM	6	5	U	Supporting
	0.500	1.50	PROPYLENE					
30-Aug-82 ONI	0.500	1.50	PROPYLENE	ETPM	7	6	U	Satisfactory
	0.500	1.50	PROPYLENE					
14-Sep-82 ONI	0.626	1.64	PROPYLENE	ETPM	7	4	S	Supporting
	0.614	1.64	PROPYLENE					

Table 17. Matched Runs, cont.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
********** For the Series				Matched propylene	**********				
21-Sep-82	ONI	0.500	1.50	PROPYLENE	ETPM	2	4	L	Supporting
		0.500	1.50	PROPYLENE					
25-Sep-82	ONI	0.300	3.00	PROPYLENE	ETPM	7	5	U	Some problems
		0.300	3.00	PROPYLENE					
19-Oct-82	ONI	0.400	3.00	PROPYLENE	ETPM	8	4	U	Some problems
		0.400	3.00	PROPYLENE					
22-Oct-82	ONI	0.500	4.00	PROPYLENE	ETPM	3	4	U	Supporting
		0.500	4.00	PROPYLENE					
1-Nov-82	ONI	0.350	4.00	PROPYLENE	ETPM	2	5	U	Supporting
		0.350	4.00	PROPYLENE					
8-Nov-82	ONI	0.350	4.00	PROPYLENE	ETPM	8	4	U	Not for model
		0.350	4.00	PROPYLENE					
23-Nov-82	ONI	0.500	4.00	PROPYLENE	ETPM	2	6	U	Some problems
		0.500	4.00	PROPYLENE					
10-Jun-83	ONI	0.500	3.00	PROPYLENE	ETPM	5	4	L	Satisfactory
		0.500	3.00	PROPYLENE					
18-Jun-83	ONI	0.537	1.00	PROPYLENE	ETPM	5	6	L	Satisfactory
		0.538	1.00	PROPYLENE					
20-Jul-83	ONI	0.242	1.15	PROPYLENE	ETPM	9	5	L	Satisfactory
		0.229	1.15	PROPYLENE					

Table 17. Matched Runs, cont.

```
   RUN
   DATE          NOx   HC                         Proj Q I P     GUIDE

********** For the Series   Matched propylene          **********

  5-Sep-83 ONI    0.500  1.50    PROPYLENE         ETPM 5 6 N Some problems
                  0.500  1.50    PROPYLENE

  7-Sep-83 ONI    0.500  1.50    PROPYLENE         ETPM 7 6 L Satisfactory
                  0.500  1.50    PROPYLENE

 18-Sep-83 ONI    0.440  1.50    PROPYLENE         ETPM 8 5 P Satisfactory
                  0.440  1.50    PROPYLENE

 14-Oct-83 ONI    0.277  2.50    PROPYLENE         ETPM 5 7 L Satisfactory
                  0.274  2.50    PROPYLENE

Number of runs for this type HC is    33

Number of runs for this Series is    33
```

Table 17. Matched Runs, cont.

```
 RUN
 DATE            NOx    HC                            Proj Q I P     GUIDE

********** For the Series   Matched mixture              **********

>>>>>>>>>>  For the HC type of   MB  Mixture, simple       <<<<<<<<<<

  7-Sep-79 ONI     0.547  0.09   ETHYLENE             ETPM 5 0 S Best of kind
                          1.25   FORMALDEHYDE
                   0.549  0.06   ETHYLENE
                          1.25   FORMALDEHYDE

  1-Aug-80 ONI     0.533  0.48   ETHYLENE             ETPM 9 0 S Best of kind
                          0.23   TRANS-2-BUTENE
                   0.551  0.46   ETHYLENE
                          0.23   TRANS-2-BUTENE

 14-Aug-80 ONI     0.470  0.91   ETHYLENE             ETPM 6 0 S Satisfactory
                          0.29   TRANS-2-BUTENE
                   0.466  0.95   ETHYLENE
                          0.32   TRANS-2-BUTENE

 12-Jun-83 ONI     0.280  2.76   BUTANE/PROPYLENE     REAC 8 2 P Best of kind
                   0.280  2.76   BUTANE/PROPYLENE

Number of runs for this type HC is     4
```

Table 17. Matched Runs, cont.

```
   RUN
   DATE           NOx    HC                        Proj Q I P      GUIDE

********** For the Series   Matched mixture            **********

>>>>>>>>>>  For the HC type of   MC  Mixture, complex      <<<<<<<<<<

  6-Jul-81 ONI    0.200  2.00     UNCMIX               ETPM 1 4 N Not for model
                  0.200  2.00     UNCMIX

 19-Sep-81 ONI    0.235  1.40     UNCMIX               ETPM 8 2 L Best of kind
                  0.235  1.40     UNCMIX

 18-Nov-81 ONI    0.200  2.00     UNCMIX               ETPM 1 6 N Not for model
                  0.200  2.00     UNCMIX

  9-Sep-82 ONI    0.300  2.00     UNCMIX               ETPM 7 4 U Best of kind
                  0.300  2.00     UNCMIX

 28-Sep-82 ONI    0.350  3.00     UNCMIX               ETPM 8 5 U Supporting
                  0.350  3.00     UNCMIX

 10-Jul-83 ONI    0.350  1.11     SIMMIX2              REAC 6 5 L Best of kind
                         0.57     BUTANE/PROPYLENE
                         0.56     TOL/XYL/MIX1
                  0.350  1.11     SIMMIX2
                         0.57     BUTANE/PROPYLENE
                         0.56     TOL/XYL/MIX1

Number of runs for this type HC is     6

Number of runs for this Series is    10
```

Table 17. Matched Runs, cont.

```
    RUN
    DATE           NOx    HC                          Proj Q I P      GUIDE

********** For the Series   Matched other              **********

>>>>>>>>>>  For the HC type of   1A  Single, aldehydes     <<<<<<<<<<

 22-Nov-81 ONI    0.259  0.76    ACETALDEHYDE       ETPM 8 5 S Best of kind
                  0.263  0.81    ACETALDEHYDE

Number of runs for this type HC is     1

>>>>>>>>>>  For the HC type of   1O  Single, olefins       <<<<<<<<<<

 23-Aug-78 ONI    0.507  2.93    ETHYLENE           ETPM 8 0 S Best of kind .
                  0.521  2.97    ETHYLENE

 25-Jul-80 ONI    0.247  1.02    A-PINENE           ETPM 7 0 S Satisfactory
                  0.252  0.94    A-PINENE

Number of runs for this type HC is     2
```

Table 17. Matched Runs, cont.

```
   RUN
   DATE           NOx    HC                         Proj Q I P     GUIDE

********** For the Series   Matched other             **********

>>>>>>>>>>  For the HC type of   1P  Single, paraffins     <<<<<<<<<<

 20-Jun-83 ONI    0.504  1.00    3-PENTANONE        ETPM 4 6 P Best of kind
                  0.509  1.00    3-PENTANONE

Number of runs for this type HC is     1

>>>>>>>>>>  For the HC type of   MB Mixture, simple        <<<<<<<<<<

 21-Jul-82 ONI    0.300  3.00    CO                 ETPM 8 0 U Not for model
                         4.00    PROPYLENE
                  0.300  3.00    CO
                         4.00    PROPYLENE

Number of runs for this type HC is     1
```

Table 17. Matched Runs, cont.

********** For the Series   Matched other   **********

>>>>>>>>>> For the HC type of   MC Mixture, complex   <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
25-Jun-82	ONI	0.617	0.55	'79 VOLARE AUTO EXHAUST DIRECT	AUTO	8	6	S	Satisfactory
		0.648	0.55	'79 VOLARE AUTO EXHAUST DIRECT					
29-Jun-82	ONI	0.244	2.46	'79 VOLARE AUTO EXHAUST DIRECT	AUTO	8	6	S	Satisfactory
		0.260	2.48	'79 VOLARE AUTO EXHAUST DIRECT					
30-Jun-82	ONI	0.329	3.13	'79 VOLARE AUTO EXHAUST DIRECT	AUTO	9	6	S	Satisfactory
		0.327	2.84	'79 VOLARE AUTO EXHAUST DIRECT					
1-Jul-82	ONI	0.369	3.53	'72 DODGE AUTO EXHAUST DIRECT	AUTO	9	6	S	Satisfactory
		0.352	3.60	'72 DODGE AUTO EXHAUST DIRECT					
10-Jul-82	ONI	0.140	1.50	'72 DODGE AUTO EXHAUST DIRECT	AUTO	2	6	N	Not for model
		0.140	1.50	'72 DODGE AUTO EXHAUST DIRECT					
20-Jul-82	ONI	0.061	1.05	'72 DODGE AUTO EXHAUST DIRECT	AUTO	5	6	N	Not for model
		0.061	1.95	'72 DODGE AUTO EXHAUST CRYO					

Table 17. Matched Runs, cont.

RUN DATE	NOx	HC		Proj Q I P	GUIDE
********** For the Series Matched other **********					
5-Aug-82 ONI	0.380	1.55	'72 DODGE AUTO EXHAUST DIRECT	AUTO 4 6 N	Not for model
	0.380	1.44	'72 DODGE AUTO EXHAUST CRYO		
6-Aug-82 ONI	0.374	1.38	'72 DODGE AUTO EXHAUST DIRECT	AUTO 8 7 S	Satisfactory
	0.358	1.07	'72 DODGE AUTO EXHAUST CRYO		
7-Aug-82 ONI	0.293	1.48	'72 DODGE AUTO EXHAUST DIRECT	AUTO 7 5 S	Satisfactory
	0.289	1.45	'72 DODGE AUTO EXHAUST CRYO		
11-Aug-82 ONI	0.300	3.00	'72 DODGE AUTO EXHAUST DIRECT	AUTO 3 7 N	Not for model
	0.300	3.00	'72 DODGE AUTO EXHAUST CRYO		
17-Sep-82 ONI	0.255	2.16	'72 DODGE AUTO EXHAUST DIRECT	AUTO 7 6 S	Satisfactory
	0.254	2.42	'72 DODGE AUTO EXHAUST CRYO		
25-Jun-83 ONI	0.301	3.00	SIMMIX2	REAC 5 5 L	Satisfactory
	0.292	3.00	SIMMIX2		

Table 17. Matched Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
15-Jul-83 ONI	0.359	2.19	'72 DODGE AUTO EXHAUST DIRECT	AUTO	9	7	S	Satisfactory
	0.352	2.25	'72 DODGE AUTO EXHAUST DIRECT					
22-Jul-83 ONI	0.267	1.81	'72 DODGE AUTO EXHAUST DIRECT	AUTO	4	7	N	Not for model
	0.274	1.86	'72 DODGE AUTO EXHAUST DIRECT					
25-Jul-83 ONI	0.235	2.96	SYNTHETIC AUTO EXHAUST 0	AURE	7	6	N	Some problems
	0.222	2.84	SYNTHETIC AUTO EXHAUST 0					
28-Jul-83 ONI	0.294	2.50	'72 DODGE AUTO EXHAUST DIRECT	AUTO	9	8	N	Satisfactory
	0.291	2.52	'72 DODGE AUTO EXHAUST DIRECT					

Number of runs for this type HC is 16

Number of runs for this Series is 21

Total number of runs is 64

Reactivity Comparison Runs

Table 18.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
********** For the Series			Reactivity Comparison		**********				
>>>>>>>>>> For the HC type of			1A Single, aldehydes		<<<<<<<<<<				
18-May-77	ONI	0.359	1.87	ACETALDEHYDE	ETPM	8	0	S	Supporting
		0.357	1.10	FORMALDEHYDE					
18-Jul-77	ONI	0.539	1.21	FORMALDEHYDE	ETPM	9	0	S	Best of HC type
		0.535	1.00	ACETALDEHYDE					
27-Jul-77	ONI	0.552	1.00	FORMALDEHYDE	ETPM	5	0	S	Supporting
		0.550	0.55	ACETALDEHYDE					
1-Aug-79	ONI	0.349	1.91	ACETALDEHYDE	ETPM	8	0	S	Best of kind
		0.353	1.00	FORMALDEHYDE					
9-Jul-80	ONI	0.746	1.70	BIACETYL	ETPM	5	0	S	Satisfactory
		0.751	1.50	METHYLGLYOXAL					
8-Aug-80	ONI	0.419	1.90	ACETALDEHYDE	ETPM	9	0	S	Best of HC type
		0.419	0.85	BIACETYL					
31-Jul-81	ONI	0.500	1.50	METHYLVINYLKETONE	ETPM	7	5	P	Satisfactory
		0.500	1.50	METHACROLEIN					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
5-Aug-81 ONI	0.443	1.60	METHACROLEIN	ETPM	8	4	S	Best of kind
	0.446	1.51	METHYLVINYLKETONE					
13-Aug-81 ONI	0.467	1.99	METHYLVINYLKETONE	ETPM	6	5	S	Best of kind
	0.469	1.90	METHACROLEIN					
14-Aug-81 ONI	0.284	1.00	METHYLVINYLKETONE	ETPM	7	5	S	Best of kind
	0.281	1.50	METHACROLEIN					
28-Sep-81 ONI	0.220	1.80	METHYLGLYOXAL	ETPM	6	5	S	Satisfactory
	0.585	1.50	BIACETYL					
1-Oct-81 ONI	0.500	1.00	BIACETYL	ETPM	8	7	S	Satisfactory
	0.500	1.00	METHYLGLYOXAL					
14-Jun-82 ONI	0.312	3.08	ACETALDEHYDE	ETPM	7	5	S	Best of kind
	0.300	3.06	PROPIONALDEHYDE					
24-Aug-82 ONI	0.336	2.07	PROPIONALDEHYDE	ETPM	8	5	S	Best of kind
	0.319	1.90	ACETALDEHYDE					
1-Oct-82 ONI	0.795	1.72	METHYLGLYOXAL	ETPM	7	6	S	Satisfactory
	0.778	1.50	GLYCOALDEHYDE					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
28-Oct-82 ONI	0.501	1.00	BIACETYL	ETPM	8	7	S	Satisfactory
	0.487	1.00	METHYLGLYOXAL					
12-Nov-82 ONI	0.000			ETPM	7	5	U	Some problems
	0.250	5.00	METHYLGLYOXAL					
23-Jun-83 ONI	0.534	1.00	METHYLGLYOXAL	ETPM	9	6	P	Satisfactory
	0.530	1.00	BIACETYL					
14-Jul-83 ONI	0.461	1.00	METHYLGLYOXAL	ETPM	7	6	P	Best of kind
	0.442	1.00	BIACETYL					

Number of runs for this type HC is 19

Table 18. Reactivity Comparison Runs, cont.

>>>>>>>>>> For the HC type of 10 Single, olefins <<<<<<<<<<

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
10-Jan-78 ONI	0.462	3.25	PROPYLENE	ETPM	8	0	S	Satisfactory
	0.482	4.35	ETHYLENE					
16-Jun-78 ONI	0.634	3.95	ETHYLENE	ETPM	7	0	S	Satisfactory
	0.640	2.00	PROPYLENE					
1-Jul-78 ONI	0.887	1.45	ETHYLENE	ETPM	7	0	S	Best of kind
	0.935	1.51	PROPYLENE					
30-Jul-78 ONI	0.474	1.32	ETHYLENE	ETPM	6	0	S	Satisfactory
	0.483	1.25	PROPYLENE					
6-Aug-78 ONI	0.561	1.69	PROPYLENE	ETPM	4	0	S	Some problems
	0.569	2.59	ETHYLENE					
15-Aug-78 ONI	0.543	1.45	PROPYLENE	ETPM	7	0	S	Best of kind
	0.563	1.58	ETHYLENE					
21-Aug-78 ONI	0.978	1.39	ETHYLENE	ETPM	9	0	S	Satisfactory
	0.981	1.28	PROPYLENE					
18-Oct-78 ONI	0.456	3.12	ETHYLENE	ETPM	9	0	S	Satisfactory
	0.456	1.52	PROPYLENE					
7-Nov-78 ONI	0.441	1.37	PROPYLENE	ETPM	5	0	S	Satisfactory
	0.441	2.67	ETHYLENE					
24-Jun-81 ONI	0.430	1.58	ISOPRENE	ETPM	8	6	P	Best of kind
	0.433	1.52	PROPYLENE					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
8-Jul-81 ONI	0.500	2.00	ISOPRENE	ETPM	7	4	L	Satisfactory
	0.500	2.00	ETHYLENE					
23-Sep-83 ONI	0.413	1.50	1-BUTENE	REAC	7	6	P	Satisfactory
	0.376	1.50	PROPYLENE					
27-Sep-83 ONI	0.473	1.50	1-BUTENE	REAC	9	5	P	Satisfactory
	0.440	1.50	TRANS-2-BUTENE					
2-Oct-83 ONI	0.456	3.31	1-BUTENE	ETPM	7	5	L	Satisfactory
	0.430	2.98	PROPYLENE					

Number of runs for this type HC is 14

Table 18. Reactivity Comparison Runs, cont.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of				1P Single, paraffins <<<<<<<<<<					
9-Oct-79	ONI	0.207	14.30	N-BUTANE	ETPM	8	0	S	Satisfactory
		0.207	14.20	N-PENTANE					
18-Oct-79	ONI	0.202	15.90	2,3-DIMETHYLBUTANE	ETPM	7	0	S	Satisfactory
		0.201	13.80	N-BUTANE					
3-Sep-82	ONI	0.230	5.07	N-PROPYLNITRATE	ETPM	8	4	S	Best of kind
		0.229	5.07	N-BUTYLNITRATE					
19-Aug-83	ONI	0.380	4.62	ISOPENTANE	ETPM	8	8	P	Best of HC type
		0.375	4.01	2,2,4-TRIMETHYLPENTANE					

Number of runs for this type HC is 4

Table 18. Reactivity Comparison Runs, cont.

>>>>>>>>>> For the HC type of 1R Single, aromatics <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
15-Aug-79	ONI	0.322	4.99	O-XYLENE	ETPM	5	0	S	Satisfactory
		0.320	5.20	TOLUENE					
30-Jul-80	ONI	0.179	3.78	TOLUENE	ETPM	7	0	S	Satisfactory
		0.178	2.23	O-XYLENE					
27-Aug-82	ONI	0.434	1.99	O-XYLENE	ETPM	8	7	S	Supporting
		0.431	3.00	TOLUENE					
27-Oct-82	ONI	0.400	4.50	TOLUENE	ETPM	8	7	S	Satisfactory
		0.399	2.78	O-XYLENE					
1-Aug-83	ONI	0.395	4.59	TOLUENE	ETPM	8	8	P	Best of HC type
		0.372	2.62	O-XYLENE					
8-Aug-83	ONI	0.434	6.00	O-XYLENE	ETPM	5	7	L	Satisfactory
		0.421	9.00	TOLUENE					
9-Aug-83	ONI	0.347	4.00	1,2,4-TRIMETHYLBENZENE	ETPM	5	9	L	Best of kind
		0.334	4.00	M-ETHYLTOLUENE					

Number of runs for this type HC is 7

Table 18. Reactivity Comparison Runs, cont.

>>>>>>>>>> For the HC type of 1U Single, ole vs ald <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
12-Nov-77	ONI	0.503	2.00	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.471	1.72	ACETALDEHYDE					
19-Nov-77	ONI	0.451	3.78	ETHYLENE	ETPM	7	0	S	Satisfactory
		0.832	3.82	ACETALDEHYDE					
20-Nov-77	ONI	0.446	4.37	ETHYLENE	ETPM	8	0	S	Satisfactory
		0.881	3.92	ACETALDEHYDE					
26-Dec-77	ONI	0.399	2.96	PROPYLENE	ETPM	9	0	S	Satisfactory
		0.407	3.82	ACETALDEHYDE					
27-Feb-78	ONI	0.496	3.95	PROPYLENE	ETPM	7	0	S	Satisfactory
		0.354	1.90	ACETALDEHYDE					
6-Mar-78	ONI	0.511	3.77	PROPYLENE	ETPM	5	0	S	Supporting
		0.374	1.80	ACETALDEHYDE					
31-Mar-78	ONI	0.483	3.82	PROPYLENE	ETPM	6	0	S	Supporting
		0.393	2.00	ACETALDEHYDE					
19-Sep-78	ONI	0.688	1.88	ETHYLENE	ETPM	7	0	S	Supporting
		0.690	2.00	FORMALDEHYDE					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
21-Sep-78 ONI	0.258	1.93	ETHYLENE	ETPM	5	0	S	Supporting
	0.257	1.97	FORMALDEHYDE					
31-Jul-79 ONI	0.513	1.43	FORMALDEHYDE	ETPM	7	0	S	Supporting
	0.513	5.13	PROPYLENE					
2-Aug-79 ONI	0.205	1.49	PROPYLENE	ETPM	7	0	S	Best of kind
	0.205	1.01	FORMALDEHYDE					
4-Aug-79 ONI	0.227	0.88	ETHYLENE	ETPM	6	0	S	Satisfactory
	0.230	0.56	FORMALDEHYDE					
5-Aug-79 ONI	0.638	4.11	ETHYLENE	ETPM	5	0	S	Best of kind
	0.539	1.20	FORMALDEHYDE					
23-Jul-81 ONI	0.500	1.50	ISOPRENE	ETPM	7	4	P	Satisfactory
	0.500	1.50	FORMALDEHYDE					

Number of runs for this type HC is 14

Table 18. Reactivity Comparison Runs, cont.

```
  RUN
  DATE          NOx    HC                          Proj Q I P      GUIDE

>>>>>>>>>>  For the HC type of   1V  Single, ole vs par    <<<<<<<<<<

 22-Oct-77 ONI    0.518  3.69    PROPYLENE         ETPM 6 0 S Best of HC type
                  0.525  8.10    N-BUTANE

 24-Oct-77 ONI    0.517  3.69    PROPYLENE         ETPM 5 0 S Satisfactory
                  0.490  8.00    N-BUTANE

Number of runs for this type HC is     2


>>>>>>>>>>  For the HC type of   1W  Single, ole vs aro    <<<<<<<<<<

 16-Aug-78 ONI    0.687  1.56    PROPYLENE         ETPM 7 0 S Best of kind
                  0.691  3.93    TOLUENE

 14-Sep-78 ONI    0.292  2.24    TOLUENE           ETPM 5 0 S Satisfactory
                  0.294  0.97    ETHYLENE

 18-Sep-78 ONI    0.503  2.98    ETHYLENE          ETPM 5 0 S Supporting
                  0.496  4.21    TOLUENE

Number of runs for this type HC is     3
```

Table 18. Reactivity Comparison Runs, cont.

>>>>>>>>>> For the HC type of 1X Single, other cross <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
20-Jun-79	ONI	0.187	6.23	N-BUTANE	ETPM	6	0	S	Best of kind
		0.182	6.00	METHYL ETHYL KETONE					
27-Jun-79	ONI	0.337	5.85	BENZALDEHYDE	ETPM	6	0	S	Best of kind
		0.333	15.50	TOLUENE					
20-Oct-79	ONI	0.224	12.10	2,3-DIMETHYLBUTANE	ETPM	5	0	S	Best of kind
		0.223	13.50	METHYL ETHYL KETONE					
11-Dec-79	ONI	0.239	12.50	2,3-DIMETHYLBUTANE	ETPM	9	0	S	Satisfactory
		0.242	14.10	ACETONE					
4-Jun-80	ONI	0.176	4.80	ACETALDEHYDE	ETPM	9	0	S	Best of kind
		0.176	3.80	METHYL ETHYL KETONE					
12-Jun-80	ONI	0.221	10.90	N-BUTYLNITRATE	ETPM	7	0	S	Supporting
		0.000							
28-Jun-83	ONI	0.322	3.00	ACETONITRILE	ETPM	7	4	L	Satisfactory
		0.319	3.00	METHANOL					

Number of runs for this type HC is 7

Table 18. Reactivity Comparison Runs, cont.

>>>>>>>>>> For the HC type of MB Mixture, simple <<<<<<<<<<

RUN DATE		NOx	HC		Proj Q I P	GUIDE
3-Oct-78	ONI	0.497	0.98	ETHYLENE	ETPM 6 0 S	Satisfactory
		0.492	0.14	N-BUTANE		
			1.36	PROPYLENE		
12-Oct-78	ONI	0.479	0.20	ETHYLENE	ETPM 9 0 S	Satisfactory
			1.26	ACETALDEHYDE		
		0.479	1.33	PROPYLENE		
25-Oct-78	ONI	0.444	0.20	ETHYLENE	ETPM 9 0 S	Satisfactory
			1.16	ACETALDEHYDE		
		0.442	1.22	PROPYLENE		
16-Aug-79	ONI	0.443	1.42	PROPYLENE	ETPM 9 0 S	Best of kind
		0.436	0.17	ETHYLENE		
			1.30	ACETALDEHYDE		
27-Aug-80	ONI	0.482	2.25	TOLUENE	ETPM 8 0 S	Best of kind
			99.99	CO		
		0.491	1.91	PROPYLENE		
			99.99	CO		
9-Jun-82	ONI	0.290	1.98	N-BUTANE	REAC 7 2 S	Best of kind
			0.64	PROPYLENE		
			0.50	M-XYLENE		
		0.284	1.96	N-BUTANE		
			0.62	PROPYLENE		
			0.53	TOLUENE		

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj Q I P	GUIDE
6-Sep-82 ONI	0.456	2.33	TOLUENE	ETPM 9 5 S	Best of kind
		0.54	O-XYLENE		
	0.447	1.90	TOLUENE		
		1.05	O-XYLENE		
7-Sep-82 ONI	0.471	2.48	TOLUENE	ETPM 8 6 S	Best of kind
		0.42	O-XYLENE		
	0.462	2.00	TOLUENE		
		1.02	O-XYLENE		
8-Sep-82 ONI	0.480	3.01	TOLUENE	ETPM 7 7 S	Supporting
		1.70	O-XYLENE		
	0.475	3.80	TOLUENE		
		0.89	O-XYLENE		
16-Sep-83 ONI	0.228	0.43	ETHYLENE	REAC 5 7 P	Best of kind
		1.57	1-BUTENE		
		1.00	PROPYLENE		
	0.208	0.84	ETHYLENE		
		1.02	1-BUTENE		
		1.04	PROPYLENE		
15-Oct-83 ONI	0.481	1.13	PROPYLENE	REAC 8 5 P	Best of kind
		0.44	ETHYLENE		
		1.60	1-BUTENE		
	0.497	1.00	PROPYLENE		
		0.88	ETHYLENE		
		1.10	1-BUTENE		

Number of runs for this type HC is 11

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj Q I P	GUIDE
>>>>>>>>>> For the HC type of			MC Mixture, complex	<<<<<<<<<<	
18-Jun-78 ONI	0.354	2.27	N-BUTANE	ETPM 7 0 S	Best of kind
		0.75	PROPYLENE		
	0.354	3.28	UNCMIX		
21-Jun-78 ONI	0.357	1.85	UNCMIX	ETPM 6 0 S	Best of kind
	0.353	1.58	N-BUTANE		
		0.54	PROPYLENE		
20-Jul-81 ONI	0.500	1.40	UNCMIX	REAC 6 4 L	Best of kind
		0.60	M-XYLENE		
	0.500	1.40	UNCMIX		
		0.60	TOLUENE		
25-Aug-81 ONI	0.000	1.40	UNCMIX	REAC 8 2 L	Satisfactory
		0.60	SIMARO		
	0.300	1.40	SIMMIX1		
		0.60	SIMARO		
26-Aug-81 ONI	0.711	1.46	UNCMIX	REAC 8 5 S	Best of kind
		0.56	SIMARO		
	0.235	1.37	SIMMIX1		
		0.58	SIMARO		
31-Aug-81 ONI	0.239	2.04	SIMMIX1	REAC 8 6 S	Best of kind
	0.236	2.09	UNCMIX		

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
2-Sep-81 ONI	0.246	2.04	UNCMIX	REAC	7	3	S	Best of kind
		0.43	SIMARO					
	0.247	1.62	UNCMIX					
		0.75	SIMARO					
14-Sep-81 ONI	0.249	1.58	UNCMIX	REAC	8	5	S	Best of kind
		0.61	M-XYLENE					
	0.247	1.65	UNCMIX					
		0.52	TOLUENE					
20-Sep-81 ONI	0.238	1.62	UNCMIX	REAC	9	3	S	Best of kind
		0.65	COMARO					
	0.229	1.57	UNCMIX					
		0.51	SIMARO					
23-Sep-81 ONI	0.300	1.40	UNCMIX	REAC	8	4	L	Satisfactory
		0.10	ACETALDEHYDE					
		0.50	TOLUENE					
	0.300	1.40	UNCMIX					
		0.10	ACETALDEHYDE					
		0.50	M-XYLENE					
29-Sep-81 ONI	0.238	1.95	UNCMIX	REAC	8	5	S	Best of kind
		0.10	ACETALDEHYDE					
		0.53	TOLUENE					
	0.245	1.98	UNCMIX					
		0.10	ACETALDEHYDE					
		0.48	M-XYLENE					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
30-Sep-81 ONI	0.300	1.40	UNCMIX	REAC	8	5	L	Best of kind
		0.60	SIMARO					
	0.300	2.00	DODGEMIX II					
3-Oct-81 ONI	0.300	2.10	UNCMIX	REAC	9	3	L	Satisfactory
		0.15	ACETALDEHYDE					
		0.75	M-XYLENE					
	0.300	2.10	UNCMIX					
		0.15	ACETALDEHYDE					
		0.75	TOLUENE					
4-Oct-81 ONI	0.300	2.10	UNCMIX	REAC	9	1	L	Satisfactory
		0.90	SIMARO					
	0.300	2.10	UNCMIX					
		0.90	COMARO					
14-Oct-81 ONI	0.277	2.60	UNCMIX	REAC	9	5	S	Best of kind
		0.15	ACETALDEHYDE					
		0.71	M-XYLENE					
	0.293	2.72	UNCMIX					
		0.15	ACETALDEHYDE					
		0.71	1,2,4-TRIMETHYLB ENZENE					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
15-Oct-81 ONI	0.300	3.00	SIMMIX1	REAC	6	3	L	Some problems
	0.300	3.00	UNCMIX					
16-Oct-81 ONI	0.300	2.10	UNCMIX	REAC	5	4	L	Supporting
		0.90	SIMARO					
	0.300	2.10	SIMMIX1					
		0.90	SIMARO					
28-Oct-81 ONI	0.500	2.73	UNCMIX	REAC	9	4	L	Not for model
		1.17	SIMARO					
		0.40	ACETALDEHYDE					
	0.500	4.00	DODGEMIX II					
29-Oct-81 ONI	0.000	2.73	UNCMIX	REAC	3	4	U	Supporting
		1.17	SIMARO					
		0.04	ACETALDEHYDE					
	0.000	4.00	DODGEMIX II					
3-Nov-81 ONI	0.421	2.73	UNCMIX	REAC	6	4	L	Not for model
		1.18	SIMARO					
		0.04	ACETALDEHYDE					
	0.421	4.00	DODGEMIX II					
13-Nov-81 ONI	0.500	2.73	UNCMIX	REAC	9	0	P	Best of kind
		1.18	SIMARO					
		0.04	ACETALDEHYDE					
	0.500	4.00	DODGEMIX II					
2-Jun-82 ONI	0.500	1.40	UNCMIX	REAC	7	5	L	Best of kind
		0.36	TOLUENE					
		0.12	M-XYLENE					
	0.500	1.40	UNCMIX					
		0.60	M-XYLENE					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
8-Jun-82 ONI	0.281	2.25	UNCMIX	REAC	7	6	S	Best of kind
		0.74	ETHYLBENZENE					
	0.281	2.28	UNCMIX					
		0.78	TOLUENE					
6-Jul-82 ONI	0.228	1.43	SIMMIX2	REAC	8	5	S	Best of kind
		0.89	N-PROPYLBENZENE					
	0.225	1.38	SIMMIX2					
		0.84	TOLUENE					
8-Jul-82 ONI	0.291	1.19	BUTANE/PROPYLENE	REAC	9	7	S	Best of kind
		0.89	SIMARO					
	0.283	1.08	BUTANE/PROPYLENE					
		1.03	COMARO					
15-Jul-82 ONI	0.566	1.71	'79 VOLARE AUTO EXHAUST DIRECT	AURE	8	6	S	Satisfactory
		0.53	M-XYLENE					
	0.576	1.88	'79 VOLARE AUTO EXHAUST DIRECT					
		0.43	TOLUENE					
19-Jul-82 ONI	0.294	2.10	UNCMIX	REAC	6	7	S	Satisfactory
		0.60	COMARO					
	0.291	2.07	SIMMIX2					
		0.60	COMARO					
22-Jul-82 ONI	0.300	3.50	SIMARO	REAC	2	5	L	Supporting
	0.300	2.90	COMARO					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
26-Jul-82	0.301	2.03	UNCMIX	REAC	8	4	S	Best of kind
		0.87	N-PROPYLBENZENE					
	0.309	2.04	UNCMIX					
		0.92	ETHYLBENZENE					
27-Jul-82 ONI	0.280	0.91	M-XYLENE	REAC	8	5	S	Best of kind
		2.20	UNCMIX					
	0.290	2.20	UNCMIX					
		0.92	N-PROPYLBENZENE					
28-Jul-82 ONI	0.298	2.13	UNCMIX	REAC	6	5	S	Best of kind
		0.88	N-PROPYLBENZENE					
	0.288	2.12	UNCMIX					
		0.88	1,2,4-TRIMETHYLBENZENE					
16-Sep-82 ONI	0.423	2.28	UNCMIX	REAC	8	6	S	Best of kind
		0.92	ETHYLBENZENE					
	0.426	2.20	UNCMIX					
		0.93	M-XYLENE					
18-Sep-82 ONI	0.384	2.19	UNCMIX	REAC	7	6	S	Best of kind
		0.91	O-XYLENE					
	0.386	2.20	UNCMIX					
		0.86	M-XYLENE					
23-Sep-82 ONI	0.400	2.10	UNCMIX	REAC	9	4	L	Some problems
		0.90	SIMARO					
	0.400	2.10	UNCMIX					
		0.90	COMARO					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
24-Sep-82 ONI	0.331	2.13	SIMMIX2	ETPM	7	6	S	Best of kind
	0.331	3.06	UNCMIX					
29-Sep-82 ONI	0.392	1.72	'72 DODGE AUTO EXHAUST DIRECT	AUTO	8	7	S	Satisfactory
	0.390	1.74	'79 VOLARE AUTO EXHAUST DIRECT					
6-Oct-82 ONI	0.467	1.97	'79 VOLARE AUTO EXHAUST DIRECT	AUTO	9	7	S	Satisfactory
	0.466	1.96	'72 DODGE AUTO EXHAUST DIRECT					
6-Nov-82 ONI	0.350	3.00	UNCMIX	REAC	9	5	U	Some problems
	0.350	3.00	SIMMIX2					
11-Nov-82 ONI	0.170	2.28	UNCMIX	REAC	8	6	S	Satisfactory
		0.90	1,2,4-TRIMETHYLBENZENE					
	0.171	2.52	UNCMIX					
		0.84	N-PROPYLBENZENE					
15-Nov-82 ONI	0.180	2.51	SIMMIX2	REAC	9	5	S	Best of kind
	0.183	2.74	UNCMIX					
17-Jun-83 ONI	0.618	1.09	'72 DODGE AUTO EXHAUST DIRECT	AUTO	4	8	N	Supporting
	0.629	2.40	'79 VOLARE AUTO EXHAUST DIRECT					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
2-Jul-83 TNI	0.178	1.64	'72 DODGE AUTO EXHAUST DIRECT	AUTO	8	7	S	Best of kind
	0.184	1.70	'79 VOLARE AUTO EXHAUST DIRECT					
3-Jul-83 SNI	0.000		TWO DAY CON'T	AUTO	9	7	S	Best of kind
	0.000		TWO DAY CON'T					
8-Jul-83 ONI	0.372	1.73	'72 DODGE AUTO EXHAUST DIRECT	AUTO	9	7	P	Satisfactory
	0.368	1.69	'79 VOLARE AUTO EXHAUST DIRECT					
11-Jul-83 ONI	0.280	1.20	PROPYLENE	REAC	9	5	P	Best of kind
		1.80	SIMMIX2					
	0.265	3.00	SIMMIX2					
2-Sep-83 ONI	0.276	3.00	'72 DODGE AUTO EXHAUST DIRECT	AURE	4	9	N	Some problems
	0.278	2.40	SYNTHETIC AUTO EXHAUST 1A					
9-Sep-83 ONI	0.296	2.80	'72 DODGE AUTO EXHAUST DIRECT	AURE	7	9	U	Supporting
	0.298	2.06	SYNTHETIC AUTO EXHAUST 1A					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
20-Sep-83 ONI	0.250	2.94	'72 DODGE AUTO EXHAUST DIRECT	AUTO	4	9	N	Supporting
	0.249	2.40	SYNTHETIC AUTO EXHAUST 1B					
4-Oct-83 ONI	0.254	2.59	'72 DODGE AUTO EXHAUST DIRECT	AUTO	9	8	S	Best of kind
	0.251	2.19	SYNTHETIC AUTO EXHAUST 1B					
7-Oct-83 ONI	0.334	1.89	UNCMIX	AURE	8	8	S	Best of kind
		0.75	COMARO					
	0.345	2.69	SYNTHETIC AUTO EXHAUST 1A					
19-Oct-83 ONI	0.834	0.35	'72 DODGE AUTO EXHAUST DIRECT	AUTO	7	8	U	Supporting
	0.836	0.35	'79 VOLARE AUTO EXHAUST DIRECT					
28-Oct-83 ONI	0.279	2.40	'79 VOLARE AUTO EXHAUST DIRECT	AUTO	5	9	U	Supporting
	0.258	2.37	'72 DODGE AUTO EXHAUST DIRECT					

Table 18. Reactivity Comparison Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
2-Nov-83 TNI	0.273	1.56	'79 VOLARE AUTO EXHAUST DIRECT	AUTO	7	9	U	Supporting
	0.272	1.50	'72 DODGE AUTO EXHAUST DIRECT					
3-Nov-83 SNI	0.000		TWO DAY CON'T	AUTO	8	9	U	Supporting
	0.000		TWO DAY CON'T					

Number of runs for this type HC is 54

Number of runs for this Series is 135

Total number of runs is 135

Substitution Runs

Table 19.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
********** For the Series		Substitution, UNCMIX		**********				
25-Jun-81 ONI	0.200	1.60	UNCMIX	REAC	8	6	P	Best of kind
		0.40	ISOPRENE					
	0.200	2.00	UNCMIX					
29-Jun-81 ONI	0.200	1.38	UNCMIX	REAC	9	6	P	Best of kind
		0.29	TOLUENE					
	0.200	1.71	UNCMIX					
9-Jul-81 ONI	0.500	2.00	UNCMIX	REAC	7	5	L	Supporting
	0.500	1.40	UNCMIX					
		0.60	M-XYLENE					
22-Jul-81 ONI	0.300	2.00	UNCMIX	REAC	8	4	U	Supporting
	0.300	1.40	UNCMIX					
		0.60	M-XYLENE					
11-Aug-81 ONI	0.300	2.00	UNCMIX	REAC	3	5	L	Best of kind
	0.300	1.40	UNCMIX					
		0.60	M-XYLENE					
15-Jun-82 ONI	0.320	3.40	UNCMIX	REAC	8	7	S	Best of kind
	0.312	2.54	UNCMIX					
		0.86	COMARO					

Table 19. Substitution Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
2-Nov-82 ONI	0.350	3.00	UNCMIX	REAC	8	7	U	Supporting
	0.350	2.10	UNCMIX					
		0.90	COMARO					
7-Dec-82 ONI	0.187	2.47	UNCMIX	REAC	9	6	S	Supporting
		0.90	COMARO					
	0.186	3.49	UNCMIX					

Number of runs for this Series is 8

********** For the Series Substitution, Propylene/Butane **********

15-Jul-81 ONI	0.300	1.40	N-BUTANE	REAC	7	4	P	Satisfactory
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.60	TOLUENE					
18-Jul-81 TNI	0.300	1.40	N-BUTANE	REAC	8	5	P	Best of kind
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.62	M-XYLENE					

Table 19. Substitution Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
19-Jul-81 SNI	0.300	1.40	N-BUTANE	ETPM	8	5	P	Best of kind
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.60	M-XYLENE					
22-Sep-81 ONI	0.300	1.40	N-BUTANE	REAC	9	4	L	Satisfactory
		0.60	PROPYLENE					
	0.300	0.42	PROPYLENE					
		0.98	N-BUTANE					
		0.60	TOLUENE					
24-Sep-81 ONI	0.235	1.28	N-BUTANE	REAC	8	5	S	Satisfactory
		0.52	PROPYLENE					
	0.233	0.89	N-BUTANE					
		0.36	PROPYLENE					
		0.77	TOLUENE					

Number of runs for this Series is 5

Table 19. Substitution Runs, cont.

```
********** For the Series   Substitution, SIMMIX        **********

 21-Aug-81 ONI     0.300  2.00     SIMMIX1            REAC 7 5 L Supporting
                   0.300  1.40     SIMMIX1
                          0.60     SIMARO

 27-Aug-81 ONI     0.234  2.11     SIMMIX1            REAC 7 4 S Best of kind
                   0.233  1.43     SIMMIX1
                          0.58     SIMARO

Number of runs for this Series is     2


********** For the Series   Substitution, OTHER         **********

  9-Aug-80 ONI     0.478 40.00     ACETONE            ETPM 7 0 S Best of kind
                   0.467 36.46     ACETONE
                          1.00     FORMALDEHYDE

 13-Aug-80 ONI     0.532 22.50     METHYL ETHYL       ETPM 8 0 S Best of kind
                                   KETONE
                   0.253 18.46     METHYL ETHYL
                                   KETONE
                          0.98     FORMALDEHYDE
```

Table 19. Substitution Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
********** For the Series			Substitution, Other					**********
3-Sep-81 ONI	0.235	1.78	UNCMIX	REAC	7	4	S	Best of kind
		0.53	SIMARO					
	0.231	1.40	UNCMIX					
		0.46	SIMARO					
		0.57	PROPYLENE					
10-Sep-81 ONI	0.235	2.79	UNCMIX	REAC	7	3	S	Best of kind
		0.70	SIMARO					
	0.246	1.02	UNCMIX					
		0.50	SIMARO					
		2.21	N-BUTANE					
12-Sep-81 ONI	0.251	1.68	UNCMIX	REAC	7	4	S	Best of kind
		0.55	SIMARO					
	0.285	1.14	UNCMIX					
		0.39	SIMARO					
		0.62	N-BUTANE					

Number of runs for this Series is 5

Total number of runs is 20

Addition Runs

Table 20.

```
    RUN
    DATE          NOx    HC                           Proj Q I P     GUIDE


********** For the Series   Addition, one species       **********


>>>>>>>>>>  For the HC type of   MB  Mixture, simple       <<<<<<<<<<

 13-Jun-79 ONI    0.452  2.81    PROPYLENE          ETPM 7 0 S Best of kind
                  0.443  2.73    PROPYLENE
                         3.16    TOLUENE

 14-Jun-79 ONI    0.451  1.82    PROPYLENE          ETPM 7 0 S Best of kind
                  0.443  1.79    PROPYLENE
                         3.02    TOLUENE

 14-Jun-80 ONI    0.210  2.25    A-PINENE           ETPM 8 0 S Best of kind
                         0.90    ISOPRENE
                  0.212  1.70    A-PINENE

Number of runs for this type HC is     3


Number of runs for this Series is     3
```

Table 20. Addition Runs, cont.

```
  RUN
  DATE           NOx    HC                          Proj Q I P     GUIDE


********** For the Series   Addition, CO              **********

>>>>>>>>>>  For the HC type of   1A  Single, aldehydes     <<<<<<<<<<

 30-Jul-79 ONI     0.288  2.00    FORMALDEHYDE        ETPM 7 0 S Satisfactory
                         15.80    CO
                   0.292  2.00    FORMALDEHYDE

Number of runs for this type HC is     1


>>>>>>>>>>  For the HC type of   10  Single, olefins       <<<<<<<<<<

 31-May-79 ONI     0.491  2.70    PROPYLENE           ETPM 5 0 S Satisfactory
                   0.502  2.69    PROPYLENE
                         50.00    CO

  2-Jun-79 ONI     0.216  1.55    PROPYLENE           ETPM 7 0 S Best of kind
                   0.215  1.56    PROPYLENE
                         40.60    CO

 29-Jul-79 ONI     0.925  1.99    PROPYLENE           ETPM 5 0 S Satisfactory
                   0.928  1.88    PROPYLENE
                         11.98    CO

Number of runs for this type HC is     3
```

Table 20. Addition Runs, cont.

```
   RUN
   DATE          NOx    HC                         Proj Q I P     GUIDE

>>>>>>>>>>  For the HC type of   1P  Single, paraffins     <<<<<<<<<<

  7-Jul-83 ONI    0.396  1.00    3-PENTANONE       ETPM 9 5 P Best of kind
                        50.00    CO
                  0.383  1.00    3-PENTANONE

Number of runs for this type HC is     1

Number of runs for this Series is     5


********** For the Series   Addition, aldehyde          **********

  3-Jun-77 ONI    0.351  1.68    PROPYLENE         ETPM 7 0 S Best of kind
                         0.50    FORMALDEHYDE
                  0.345  1.69    PROPYLENE

 12-Jun-79 ONI    0.500  0.83    PROPYLENE         ETPM 7 0 S Best of kind
                  0.494  0.53    PROPYLENE
                         0.80    ACETALDEHYDE

 11-Aug-80 ONI    0.305  3.18    TOLUENE           ETPM 4 0 S Best of kind
                  0.318  3.14    TOLUENE
                         1.12    BENZALDEHYDE

 12-Aug-80 ONI    0.481  0.34    FORMALDEHYDE      ETPM 4 0 S Best of kind
                  0.484  1.00    FORMALDEHYDE
                         1.55    BENZALDEHYDE

Number of runs for this Series is     4
```

Table 20. Addition Runs, cont.

```
   RUN
   DATE             NOx    HC                              Proj Q I P      GUIDE


********** For the Series   Addition, Other             **********

>>>>>>>>>>  For the HC type of   MB  Mixture, simple       <<<<<<<<<<

 11-Sep-82 ONI     0.500  1.50    PROPYLENE          ETPM 5 6 U Supporting
                          5.00    N-BUTYLNITRATE
                   0.500  1.50    PROPYLENE

 12-Sep-82 ONI     0.692  1.69    PROPYLENE          ETPM 8 6 S Best of kind
                          5.00    N-BUTYLNITRATE
                   0.364  1.69    PROPYLENE

 13-Aug-83 ONI     0.217  1.15    PROPYLENE          REAC 9 6 S Satisfactory
                          0.27    OZONE
                   0.203  1.15    PROPYLENE

Number of runs for this type HC is     3


>>>>>>>>>>  For the HC type of   MC  Mixture, complex      <<<<<<<<<<

  6-Sep-83 ONI     0.244  2.02    UNCMIX             REAC 7 7 L Best of kind
                   0.230  1.83    UNCMIX
                          0.60    BENZENE

Number of runs for this type HC is     1


Number of runs for this Series is     4


Total number of runs is    16
```

Delta Concentration Runs

Table 21.

```
   RUN
   DATE            NOx    HC                           Proj Q I P     GUIDE

********** For the Series   Delta HC                  **********

>>>>>>>>>>  For the HC type of   1A  Single, aldehydes    <<<<<<<<<<

 28-Jul-77 ONI    0.526  1.16   FORMALDEHYDE      ETPM 5 0 S Not for model
                  0.529  2.20   FORMALDEHYDE

 19-Sep-77 ONI    0.382  1.00   FORMALDEHYDE      ETPM 3 0 S Not for model
                  0.386  0.68   FORMALDEHYDE

  8-Aug-78 ONI    0.516  0.91   ACETALDEHYDE      ETPM 4 0 S Supporting
                  0.527  4.00   ACETALDEHYDE

 17-Aug-78 ONI    0.701  0.96   ACETALDEHYDE      ETPM 6 0 S Best of kind
                  0.700  4.00   ACETALDEHYDE

  8-Sep-78 ONI    0.968  3.25   FORMALDEHYDE      ETPM 4 0 S Some problems
                  0.916  0.90   FORMALDEHYDE

 13-Oct-78 ONI    0.493  0.92   ACETALDEHYDE      ETPM 4 0 S Satisfactory
                  0.906  2.02   ACETALDEHYDE

Number of runs for this type HC is     6
```

Table 21. Delta Concentration Runs, cont.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of 10 Single, olefins <<<<<<<<<<									
20-Jul-77	ONI	0.270	0.65	PROPYLENE	ETPM	8	0	S	Best of kind
		0.280	1.21	PROPYLENE					
12-Oct-77	ONI	0.505	3.56	PROPYLENE	ETPM	4	0	S	Some problems
		0.501	1.72	PROPYLENE					
18-Oct-77	ONI	0.494	3.84	ETHYLENE	ETPM	6	0	S	Best of kind
		0.484	1.88	ETHYLENE					
9-Nov-77	ONI	0.529	3.77	PROPYLENE	ETPM	7	0	S	Satisfactory
		0.537	1.92	PROPYLENE					
24-Jul-78	ONI	0.959	2.97	PROPYLENE	ETPM	7	0	S	Satisfactory
		0.952	1.47	PROPYLENE					
5-Aug-78	ONI	0.248	0.83	PROPYLENE	ETPM	4	0	S	Satisfactory
		0.568	1.55	PROPYLENE					
18-Aug-78	ONI	0.495	0.74	PROPYLENE	ETPM	8	0	S	Best of kind
		0.491	2.88	PROPYLENE					
20-Oct-78	ONI	0.460	1.39	PROPYLENE	ETPM	7	0	S	Best of kind
		0.457	3.65	PROPYLENE					
29-Oct-78	ONI	0.498	1.35	PROPYLENE	ETPM	5	0	S	Supporting
		0.495	3.68	PROPYLENE					

Table 21. Delta Concentration Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
2-Nov-78 ONI	0.553	3.52	PROPYLENE	ETPM	8	0	S	Satisfactory
	0.550	1.41	PROPYLENE					
13-Aug-79 ONI	0.496	4.39	PROPYLENE	ETPM	7	0	S	Best of kind
	0.188	0.57	PROPYLENE					
15-Jun-80 ONI	0.213	1.22	A-PINENE	ETPM	6	0	S	Satisfactory
	0.219	0.80	A-PINENE					
17-Jun-80 ONI	0.192	0.50	ISOPRENE	ETPM	5	0	S	Satisfactory
	0.098	1.40	ISOPRENE					
8-Jul-80 ONI	0.754	2.10	ETHYLENE	ETPM	5	0	S	Best of kind
	0.754	3.23	ETHYLENE					
15-Jul-80 ONI	0.184	1.04	A-PINENE	ETPM	6	0	S	Best of kind
	0.188	2.68	A-PINENE					
16-Jul-80 ONI	0.186	4.01	ISOPRENE	ETPM	9	0	S	Some problems
	0.188	1.97	ISOPRENE					
17-Jul-80 ONI	0.460	2.58	ISOPRENE	ETPM	9	0	S	Best of kind
	0.466	0.98	ISOPRENE					
26-Aug-80 ONI	0.472	1.99	ETHYLENE	ETPM	8	0	S	Best of kind
	0.464	1.00	ETHYLENE					
19-Jun-81 ONI	0.500	2.00	ISOPRENE	ETPM	5	6	L	Some problems
	0.500	1.00	ISOPRENE					

Table 21. Delta Concentration Runs, cont.

```
  RUN
  DATE           NOx    HC                          Proj Q I P      GUIDE

21-Jun-81 ONI   0.500  2.00    ISOPRENE            ETPM 8 4 P Best of kind
                0.500  1.00    ISOPRENE

22-Jun-81 ONI   0.700  2.00    ISOPRENE            ETPM 8 5 N Satisfactory
                0.700  1.00    ISOPRENE

23-Jun-81 ONI   0.500  2.00    ISOPRENE            ETPM 7 7 P Satisfactory
                0.500  1.00    ISOPRENE

25-Sep-83 ONI   0.500  1.50    1-BUTENE            ETPM 7 5 P Best of kind
                0.500  3.00    1-BUTENE

Number of runs for this type HC is    23


>>>>>>>>>>  For the HC type of   1P  Single, paraffins     <<<<<<<<<<

21-Jul-78 ONI   0.243  7.30    N-BUTANE            ETPM 8 0 S Best of kind
                0.242 15.70    N-BUTANE

22-Jul-78 ONI   0.548  8.34    N-BUTANE            ETPM 8 0 S Best of kind
                0.557 17.50    N-BUTANE

25-Aug-78 ONI   0.518 13.20    N-BUTANE            ETPM 7 0 S Satisfactory
                0.518 26.60    N-BUTANE

Number of runs for this type HC is     3
```

Table 21. Delta Concentration Runs, cont.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of				MC Mixture, complex					<<<<<<<<<<
21-Jul-81	ONI	0.300	2.00	UNCMIX	REAC	8	4	U	Best of kind
		0.300	1.40	UNCMIX					
3-Aug-82	ONI	0.456	2.45	'72 DODGE AUTO EXHAUST DIRECT	AUTO	8	8	S	Satisfactory
		0.165	1.25	'72 DODGE AUTO EXHAUST CRYO					
3-Oct-82	ONI	0.250	2.75	SIMMIX2	REAC	9	5	S	Best of kind
		0.248	1.56	SIMMIX2					
29-Jun-83	ONI	0.140	2.50	'72 DODGE AUTO EXHAUST DIRECT	AUTO	5	7	U	Best of kind
		0.155	0.80	'72 DODGE AUTO EXHAUST DIRECT					
11-Aug-83	ONI	0.223	2.15	'79 VOLARE AUTO EXHAUST DIRECT	AUTO	9	8	S	Best of kind
		0.218	0.68	'79 VOLARE AUTO EXHAUST DIRECT					

Number of runs for this type HC is 5

Number of runs for this Series is 37

Table 21. Delta Concentration Runs, cont.

```
  RUN
  DATE           NOx    HC                            Proj Q I P      GUIDE

********** For the Series   Delta NOx                  **********

>>>>>>>>>>  For the HC type of   1A  Single, aldehydes     <<<<<<<<<<

 14-Sep-77 ONI    0.397  1.05     FORMALDEHYDE        ETPM 4 0 S Best of kind
                  0.009  1.20     FORMALDEHYDE

Number of runs for this type HC is      1


>>>>>>>>>>  For the HC type of   1P  Single, paraffins     <<<<<<<<<<

 27-Jul-78 ONI    0.266 13.50     N-BUTANE            ETPM 5 0 S Some problems
                  0.509 13.20     N-BUTANE

 24-Aug-78 ONI    0.575 58.00     N-BUTANE            ETPM 9 0 S Best of kind
                  0.803 56.30     N-BUTANE


Number of runs for this type HC is      2


>>>>>>>>>>  For the HC type of   1P  Single, olefins     <<<<<<<<<<

 13-Aug-82 ONI    0.400  3.00     PROPYLENE           ETPM 5 5 U Satisfactory
                  0.500  3.00     PROPYLENE

Number of runs for this type HC is      1
```

Table 21. Delta Concentration Runs, cont.

```
    RUN
    DATE            NOx    HC                              Proj Q I P      GUIDE

********** For the Series   Delta NOx                 **********

>>>>>>>>>>  For the HC type of   1U  Single, ole vs ald    <<<<<<<<<<

 15-Sep-78 ONI    0.526  2.98    ETHYLENE            ETPM 3 0 S Some problems
                  0.268  2.00    FORMALDEHYDE

Number of runs for this type HC is     1


Number of runs for this Series is     5



Total number of runs is    42
```

Dynamic Runs

Table 22.

```
RUN
DATE            NOx    HC                              Proj Q I P     GUIDE


********** For the Series   Static to dynamic          **********

>>>>>>>>>>  For the HC type of   10  Single, olefins        <<<<<<<<<<

  9-Sep-81 ONB    0.165  1.02   ISOPRENE               ETPM 7 4 S 301
                  0.012  0.05   ISOPRENE

 29-Aug-82 ONH    0.235         PROPYLENE              ETPM 7 0 N 501
                  0.235  1.10   PROPYLENE

  4-Sep-82 ONH    0.220         PROPYLENE              ETPM 9 5 S   2
                  0.231  1.15   PROPYLENE

 10-Sep-82 ONB    0.060         PROPYLENE              ETPM 6 0 N 502
                  0.255  1.10   PROPYLENE

 13-Sep-82 ONB    0.149         PROPYLENE              ETPM 8 3 S   4
                  0.321  1.09   PROPYLENE

 17-Jul-83 ONH    0.267  1.15   PROPYLENE              ETPM 9 5 P   3
                  0.260         PROPYLENE

 21-Jul-83 ONB    0.213  1.15   PROPYLENE              ETPM 9 5 P   5
                  0.000         PROPYLENE
```

Table 22. Dynamic Runs, cont.

RUN DATE	NOx	HC		Proj Q I P	GUIDE
29-Jul-83 ODI	0.200	1.15	PROPYLENE	ETPM 9 5 P	1
	0.198	1.15	PROPYLENE		
31-Jul-83 ONB	0.200	1.15	PROPYLENE	ETPM 9 5 P	6
	0.000		PROPYLENE		

Number of runs for this type HC is 9

Table 22. Dynamic Runs, cont.

>>>>>>>>>> For the HC type of MB Mixture, simple <<<<<<<<<<

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
14-Jun-83 ONB	0.230	1.83	BUTANE/PROPYLENE	ETPM	7	5	P	10
		0.73	TOLUENE					
	0.000		BUTANE/PROPYLENE					
			TOLUENE					
27-Jun-83 ODC	0.036		BUTANE/PROPYLENE	ETPM	8	5	P	11
			TOLUENE					
	0.280	1.83	BUTANE/PROPYLENE					
		0.79	TOLUENE					
18-Aug-83 ODC	0.280	0.42	PROPYLENE	REAC	7	7	P	13
		1.41	N-BUTANE					
		0.79	TOLUENE					
	0.280	0.42	PROPYLENE					
		1.41	N-BUTANE					
		0.79	TOLUENE					
26-Aug-83 ODC	0.310	0.78	TOLUENE	ETPM	9	9	P	12
		0.42	PROPYLENE					
		1.40	N-BUTANE					
	0.110		TOLUENE					
			PROPYLENE					
			N-BUTANE					

Number of runs for this type HC is 4

Table 22. Dynamic Runs, cont.

>>>>>>>>>> For the HC type of MC Mixture, complex <<<<<<<<<<

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
12-Sep-83 ONC	0.330	1.00	UNCMIX TOL/XYL/MIX3 ISO-/2,2,4-TM-PE NTANES	REAC	8	8	P	12
	0.330	0.50	UNCMIX TOL/XYL/MIX3 ISO-/2,2,4-TM-PE NTANES					
6-Oct-83 ODI	0.367	2.10	UNCMIX	ETPM	7	8	P	20
		0.83	TOL/TMB/XYLS					
	0.365	2.10	UNCMIX					
		0.82	TOL/TMB/XYLS					

Number of runs for this type HC is 2

Table 22. Dynamic Runs, cont.

>>>>>>>>>>> For the HC type of MV Mixture, varying <<<<<<<<<<

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
9-Jul-83 ONH	0.343		SIMMIX2	REAC	8	5	P	30
		0.57	BUTANE/PROPYLENE					
		0.56	TOL/XYL/MIX1					
	0.355		SIMMIX2					
		0.57	BUTANE/PROPYLENE					
		0.56	TOL/XYL/MIX1					
22-Aug-83 ONB	0.180	0.57	BUTANE/PROPYLENE	REAC	9	9	P	32
			SIMMIX2					
		0.56	TOL/XYL/MIX1					
	0.000	0.57	BUTANE/PROPYLENE					
			SIMMIX2					
		0.56	TOL/XYL/MIX1					
17-Oct-83 ONH	0.493	1.12	PROPYLENE	REAC	9	6	P	31
		1.26	TOL/XYL/MIX2					
			ISO-/2,2,4-TM-PENTANES					
	0.493	1.12	PROPYLENE					
		1.21	TOL/XYL/MIX2					
		2.01	ISO-/2,2,4-TM-PENTANES					

Number of runs for this type HC is 3

Number of runs for this Series is 18

Total number of runs is 18

5

Runs by Species

The purpose of this chapter is to list selected experiments sorted by species. The runs sorted in this manner are listed in Tables 23–28. The species selected are: formaldehyde (Table 23), acetaldehyde (Table 24), ethylene (Table 25), propylene (other than matched propylene) (Table 26), n-butane (Table 27), and toluene (Table 28).

As in Chapter 4, within each series list, the runs are grouped by HC type beginning with the simplest type that appears in the series. Within the HC type grouping, the runs are in chronological order.

Also as in Chapter 4, codes are listed for the Class, Dilution, and Injection conditions of the runs. These were defined in Table 3. The initial conditions for NO_x and for up to three HC reactants or HC mixtures are listed. The project is identified. The run quality, number of instruments used, and the current processing status are given.

Finally, guidance for the usefulness of a specific run is given in terms of the general ranking categories that were defined in Table 15.

Formaldehyde Runs

Table 23.

>>>>>>>>>> For the HC type of 1A Single, aldehydes <<<<<<<<<<

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
18-May-77 ONI	0.359	1.87	ACETALDEHYDE	ETPM	8	0	S	Supporting
	0.357	1.10	FORMALDEHYDE					
18-Jul-77 ONI	0.539	1.21	FORMALDEHYDE	ETPM	9	0	S	Best of HC type
	0.535	1.00	ACETALDEHYDE					
27-Jul-77 ONI	0.552	1.00	FORMALDEHYDE	ETPM	5	0	S	Supporting
	0.550	0.55	ACETALDEHYDE					
28-Jul-77 ONI	0.526	1.16	FORMALDEHYDE	ETPM	5	0	S	Not for model
	0.529	2.20	FORMALDEHYDE					
14-Sep-77 ONI	0.397	1.05	FORMALDEHYDE	ETPM	4	0	S	Best of kind
	0.009	1.20	FORMALDEHYDE					
19-Sep-77 ONI	0.382	1.00	FORMALDEHYDE	ETPM	3	0	S	Not for model
	0.386	0.68	FORMALDEHYDE					
8-Sep-78 ONI	0.968	3.25	FORMALDEHYDE	ETPM	4	0	S	Some problems
	0.916	0.90	FORMALDEHYDE					
30-Jul-79 ONI	0.288	2.00	FORMALDEHYDE	ETPM	7	0	S	Satisfactory
		15.80	CO					
	0.292	2.00	FORMALDEHYDE					

Table 23. Formaldehyde Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
1-Aug-79 ONI	0.349	1.91	ACETALDEHYDE	ETPM	8	0	S	Best of kind
	0.353	1.00	FORMALDEHYDE					
17-Jul-82 CNI	0.003	0.52	FORMALDEHYDE	ETPM	8	5	S	Best of kind
	0.007	0.58	FORMALDEHYDE					

Number of runs for this type HC is 10

Table 23. Formaldehyde Runs, cont.

>>>>>>>>>> For the HC type of 1U Single, ole vs ald <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
15-Sep-78	ONI	0.526	2.98	ETHYLENE	ETPM	3	0	S	Supporting
		0.268	2.00	FORMALDEHYDE					
19-Sep-78	ONI	0.688	1.88	ETHYLENE	ETPM	7	0	S	Supporting
		0.690	2.00	FORMALDEHYDE					
21-Sep-78	ONI	0.258	1.93	ETHYLENE	ETPM	5	0	S	Supporting
		0.257	1.97	FORMALDEHYDE					
31-Jul-79	ONI	0.513	1.43	FORMALDEHYDE	ETPM	7	0	S	Supporting
		0.513	5.13	PROPYLENE					
2-Aug-79	ONI	0.205	1.49	PROPYLENE	ETPM	7	0	S	Best of kind
		0.205	1.01	FORMALDEHYDE					
4-Aug-79	ONI	0.227	0.88	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.230	0.56	FORMALDEHYDE					
5-Aug-79	ONI	0.638	4.11	ETHYLENE	ETPM	5	0	S	Best of kind
		0.539	1.20	FORMALDEHYDE					
23-Jul-81	ONI	0.500	1.50	ISOPRENE	ETPM	7	4	P	Satisfactory
		0.500	1.50	FORMALDEHYDE					

Number of runs for this type HC is 8

Table 23. Formaldehyde Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of MB Mixture, simple <<<<<<<<<<								
3-Jun-77 ONI	0.351	1.68	PROPYLENE	ETPM	7	0	S	Best of kind
		0.50	FORMALDEHYDE					
	0.345	1.69	PROPYLENE					
7-Sep-79 ONI	0.547	0.09	ETHYLENE	ETPM	5	0	S	Best of kind
		1.25	FORMALDEHYDE					
	0.549	0.06	ETHYLENE					
		1.25	FORMALDEHYDE					
9-Aug-80 ONI	0.478	40.00	ACETONE	ETPM	7	0	S	Best of kind
	0.467	36.46	ACETONE					
		1.00	FORMALDEHYDE					
12-Aug-80 ONI	0.481	0.84	FORMALDEHYDE	ETPM	4	0	S	Best of kind
	0.484	1.00	FORMALDEHYDE					
		1.55	BENZALDEHYDE					
13-Aug-80 ONI	0.532	22.50	METHYL ETHYL KETONE	ETPM	8	0	S	Best of kind
	0.253	18.46	METHYL ETHYL KETONE					
		0.98	FORMALDEHYDE					

Number of runs for this type HC is 5

Total number of runs is 23

Acetaldehyde Runs

Table 24.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>>> For the HC type of 1A Single, aldehydes <<<<<<<<<<								
18-May-77 ONI	0.359	1.87	ACETALDEHYDE	ETPM	8	0	S	Supporting
	0.357	1.10	FORMALDEHYDE					
18-Jul-77 ONI	0.539	1.21	FORMALDEHYDE	ETPM	9	0	S	Best of HC type
	0.535	1.00	ACETALDEHYDE					
27-Jul-77 ONI	0.552	1.00	FORMALDEHYDE	ETPM	5	0	S	Supporting
	0.550	0.55	ACETALDEHYDE					
8-Aug-78 ONI	0.516	0.91	ACETALDEHYDE	ETPM	4	0	S	Supporting
	0.527	4.00	ACETALDEHYDE					
17-Aug-78 ONI	0.701	0.96	ACETALDEHYDE	ETPM	6	0	S	Best of kind
	0.700	4.00	ACETALDEHYDE					
13-Oct-78 ONI	0.493	0.92	ACETALDEHYDE	ETPM	4	0	S	Satisfactory
	0.906	2.02	ACETALDEHYDE					
21-May-79 CNI	0.004	2.81	ACETALDEHYDE	ETPM	7	0	S	Satisfactory
	0.004	0.83	ACETALDEHYDE					
21-Jul-79 CNI	0.009	2.00	ACETALDEHYDE	ETPM	4	0	S	Satisfactory
	0.015	2.00	ACETALDEHYDE					

Table 24. Acetaldehyde Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
1-Aug-79 ONI	0.349	1.91	ACETALDEHYDE	ETPM	8	0	S	Best of kind
	0.353	1.00	FORMALDEHYDE					
8-Aug-80 ONI	0.419	1.90	ACETALDEHYDE	ETPM	9	0	S	Best of HC type
	0.419	0.85	BIACETYL					
22-Nov-81 CNI	0.259	0.76	ACETALDEHYDE	ETPM	8	5	S	Best of kind
	0.263	0.81	ACETALDEHYDE					
14-Jun-82 ONI	0.312	3.08	ACETALDEHYDE	ETPM	7	5	S	Best of kind
	0.300	3.06	PROPIONALDEHYDE					
24-Aug-82 ONI	0.336	2.07	PROPIONALDEHYDE	ETPM	8	5	S	Best of kind
	0.319	1.90	ACETALDEHYDE					
13-Jul-83 CNI	0.000	1.00	ACETALDEHYDE	ETPM	5	5	L	Best of kind
		0.50	CO					
	0.000	1.00	ACETALDEHYDE					

Number of runs for this type HC is 14

Table 24. Acetaldehyde Runs, cont.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of 1U Single, ole vs ald <<<<<<<<<<									
12-Nov-77	ONI	0.503	2.00	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.471	1.72	ACETALDEHYDE					
19-Nov-77	ONI	0.451	3.78	ETHYLENE	ETPM	7	0	S	Satisfactory
		0.332	3.82	ACETALDEHYDE					
20-Nov-77	ONI	0.446	4.37	ETHYLENE	ETPM	8	0	S	Satisfactory
		0.881	3.92	ACETALDEHYDE					
26-Dec-77	ONI	0.399	2.96	PROPYLENE	ETPM	9	0	S	Satisfactory
		0.407	3.82	ACETALDEHYDE					
27-Feb-78	ONI	0.496	3.95	PROPYLENE	ETPM	7	0	S	Satisfactory
		0.354	1.90	ACETALDEHYDE					
6-Mar-78	ONI	0.511	3.77	PROPYLENE	ETPM	5	0	S	Supporting
		0.374	1.80	ACETALDEHYDE					
31-Mar-78	ONI	0.483	3.82	PROPYLENE	ETPM	6	0	S	Supporting
		0.393	2.00	ACETALDEHYDE					

Number of runs for this type HC is 7

Table 24. Acetaldehyde Runs, cont.

```
RUN
DATE          NOx    HC                         Proj Q I P    GUIDE

>>>>>>>>>>  For the HC type of   1X  Single, other cross   <<<<<<<<<<

  4-Jun-80 ONI    0.176  4.80    ACETALDEHYDE       ETPM 9 0 S Best of kind
                  0.176  3.80    METHYL ETHYL
                                 KETONE

Number of runs for this type HC is     1


>>>>>>>>>>  For the HC type of   B   Background Air       <<<<<<<<<<

  7-Jun-82 DNI    0.000  1.00    ACETALDEHYDE       ETPM 8 0 S Supporting
                                 TWO DAY CON'T
                  0.000  1.00    ACETALDEHYDE
                                 TWO DAY CON'T

 26-Jul-83 CNI    0.020  0.97    ACETALDEHYDE       ETPM 7 5 P Satisfactory
                        54.90    CO
                  0.010  1.00    ACETALDEHYDE

  4-Aug-83 CNI    0.000          ACETALDEHYDE       ETPM 7 6 P Satisfactory
                        50.00    CO
                  0.000          ACETALDEHYDE

 25-Aug-83 CNI    0.000  1.00    ACETALDEHYDE       ETPM 7 6 P Satisfactory
                        50.00    CO
                  0.000  1.00    ACETALDEHYDE

Number of runs for this type HC is     4
```

Table 24. Acetaldehyde Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of MB Mixture, simple <<<<<<<<<<								
12-Oct-78 ONI	0.479	0.20	ETHYLENE	ETPM	9	0	S	Satisfactory
		1.26	ACETALDEHYDE					
	0.479	1.33	PROPYLENE					
25-Oct-78 ONI	0.444	0.20	ETHYLENE	ETPM	9	0	S	Satisfactory
		1.16	ACETALDEHYDE					
	0.442	1.22	PROPYLENE					
12-Jun-79 ONI	0.500	0.83	PROPYLENE	ETPM	7	0	S	Best of kind
	0.494	0.53	PROPYLENE					
		0.80	ACETALDEHYDE					
16-Aug-79 ONI	0.443	1.42	PROPYLENE	ETPM	9	0	S	Best of kind
	0.436	0.17	ETHYLENE					
		1.30	ACETALDEHYDE					

Number of runs for this type HC is 4

Table 24. Acetaldehyde Runs, cont.

RUN DATE	NOx	HC		Proj Q I P	GUIDE
>>>>>>>>>> For the HC type of			MC Mixture, complex	<<<<<<<<<<	
23-Sep-81 ONI	0.300	1.40	UNCMIX	REAC 8 4 L	Satisfactory
		0.10	ACETALDEHYDE		
		0.50	TOLUENE		
	0.300	1.40	UNCMIX		
		0.10	ACETALDEHYDE		
		0.50	M-XYLENE		
29-Sep-81 ONI	0.238	1.95	UNCMIX	REAC 8 5 S	Best of kind
		0.10	ACETALDEHYDE		
		0.53	TOLUENE		
	0.245	1.98	UNCMIX		
		0.10	ACETALDEHYDE		
		0.48	M-XYLENE		
3-Oct-81 ONI	0.300	2.10	UNCMIX	REAC 9 3 L	Satisfactory
		0.15	ACETALDEHYDE		
		0.75	M-XYLENE		
	0.300	2.10	UNCMIX		
		0.15	ACETALDEHYDE		
		0.75	TOLUENE		
14-Oct-81 ONI	0.277	2.60	UNCMIX	REAC 9 5 S	Best of kind
		0.15	ACETALDEHYDE		
		0.71	M-XYLENE		
	0.293	2.72	UNCMIX		
		0.15	ACETALDEHYDE		
		0.71	1,2,4-TRIMETHYLBENZENE		

Table 24. Acetaldehyde Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
28-Oct-81 ONI	0.500	2.73	UNCMIX	REAC	9	4	L	Not for model
		1.17	SIMARO					
		0.40	ACETALDEHYDE					
	0.500	4.00	DODGEMIX II					
29-Oct-81 ONI	0.000	2.73	UNCMIX	REAC	3	4	U	Supporting
		1.17	SIMARO					
		0.04	ACETALDEHYDE					
	0.000	4.00	DODGEMIX II					
3-Nov-81 ONI	0.421	2.73	UNCMIX	REAC	6	4	L	Not for model
		1.18	SIMARO					
		0.04	ACETALDEHYDE					
	0.421	4.00	DODGEMIX II					
13-Nov-81 ONI	0.500	2.73	UNCMIX	REAC	9	0	P	Best of kind
		1.18	SIMARO					
		0.04	ACETALDEHYDE					
	0.500	4.00	DODGEMIX II					

Number of runs for this type HC is 8

Total number of runs is 37

Ethylene Runs

Table 25.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of 10 Single, olefins <<<<<<<<<<									
18-Oct-77	ONI	0.494	3.84	ETHYLENE	ETPM	6	0	S	Best of kind
		0.484	1.88	ETHYLENE					
10-Jan-78	ONI	0.462	3.25	PROPYLENE	ETPM	8	0	S	Satisfactory
		0.482	4.35	ETHYLENE					
16-Jun-78	ONI	0.634	3.95	ETHYLENE	ETPM	7	0	S	Satisfactory
		0.640	2.00	PROPYLENE					
1-Jul-78	ONI	0.887	1.45	ETHYLENE	ETPM	7	0	S	Best of kind
		0.935	1.51	PROPYLENE					
30-Jul-78	ONI	0.474	1.32	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.483	1.25	PROPYLENE					
6-Aug-78	ONI	0.561	1.69	PROPYLENE	ETPM	4	0	S	Some problems
		0.569	2.59	ETHYLENE					
15-Aug-78	ONI	0.543	1.45	PROPYLENE	ETPM	7	0	S	Best of kind
		0.563	1.58	ETHYLENE					

Table 25. Ethylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
21-Aug-78 ONI	0.978	1.39	ETHYLENE	ETPM	9	0	S	Satisfactory
	0.981	1.28	PROPYLENE					
23-Aug-78 ONI	0.507	2.93	ETHYLENE	ETPM	8	0	S	Best of kind
	0.521	2.97	ETHYLENE					
18-Oct-78 ONI	0.456	3.12	ETHYLENE	ETPM	9	0	S	Satisfactory
	0.456	1.52	PROPYLENE					
7-Nov-78 ONI	0.441	1.37	PROPYLENE	ETPM	5	0	S	Satisfactory
	0.441	2.67	ETHYLENE					
8-Jul-80 ONI	0.754	2.10	ETHYLENE	ETPM	5	0	S	Best of kind
	0.754	3.23	ETHYLENE					
26-Aug-80 ONI	0.472	1.99	ETHYLENE	ETPM	8	0	S	Best of kind
	0.464	1.00	ETHYLENE					
8-Jul-81 ONI	0.500	2.00	ISOPRENE	ETPM	7	4	L	Satisfactory
	0.500	2.00	ETHYLENE					

Number of runs for this type HC is 14

Table 25. Ethylene Runs, cont.

>>>>>>>>>>> For the HC type of 1U Single, ole vs ald <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
12-Nov-77	ONI	0.503	2.00	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.471	1.72	ACETALDEHYDE					
19-Nov-77	ONI	0.451	3.78	ETHYLENE	ETPM	7	0	S	Satisfactory
		0.832	3.82	ACETALDEHYDE					
20-Nov-77	ONI	0.446	4.37	ETHYLENE	ETPM	8	0	S	Satisfactory
		0.881	3.92	ACETALDEHYDE					
15-Sep-78	ONI	0.526	2.98	ETHYLENE	ETPM	3	0	S	Supporting
		0.268	2.00	FORMALDEHYDE					
19-Sep-78	ONI	0.688	1.88	ETHYLENE	ETPM	7	0	S	Supporting
		0.690	2.00	FORMALDEHYDE					
21-Sep-78	ONI	0.258	1.93	ETHYLENE	ETPM	5	0	S	Supporting
		0.257	1.97	FORMALDEHYDE					
4-Aug-79	ONI	0.227	0.88	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.230	0.56	FORMALDEHYDE					
5-Aug-79	ONI	0.638	4.11	ETHYLENE	ETPM	5	0	S	Best of kind
		0.539	1.20	FORMALDEHYDE					

Number of runs for this type HC is 8

Table 25. Ethylene Runs, cont.

```
RUN
DATE            NOx     HC                          Proj Q I P     GUIDE

>>>>>>>>>>  For the HC type of   1W  Single, ole vs aro    <<<<<<<<<<

 14-Sep-78 ONI   0.292  2.24    TOLUENE            ETPM 5 0 S Satisfactory
                 0.294  0.97    ETHYLENE

 18-Sep-78 ONI   0.503  2.98    ETHYLENE           ETPM 5 0 S Supporting
                 0.496  4.21    TOLUENE

Number of runs for this type HC is     2

>>>>>>>>>>  For the HC type of   MB  Mixture, simple       <<<<<<<<<<

  3-Oct-78 ONI   0.497  0.98    ETHYLENE           ETPM 6 0 S Satisfactory
                 0.492  0.14    N-BUTANE
                        1.36    PROPYLENE

 12-Oct-78 ONI   0.479  0.20    ETHYLENE           ETPM 9 0 S Satisfactory
                        1.26    ACETALDEHYDE
                 0.479  1.33    PROPYLENE

 25-Oct-78 ONI   0.444  0.20    ETHYLENE           ETPM 9 0 S Satisfactory
                        1.16    ACETALDEHYDE
                 0.442  1.22    PROPYLENE

 16-Aug-79 ONI   0.443  1.42    PROPYLENE          ETPM 9 0 S Best of kind
                 0.436  0.17    ETHYLENE
                        1.30    ACETALDEHYDE

  7-Sep-79 ONI   0.547  0.09    ETHYLENE           ETPM 5 0 S Best of kind
                        1.25    FORMALDEHYDE
                 0.549  0.06    ETHYLENE
                        1.25    FORMALDEHYDE
```

Table 25. Ethylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
1-Aug-80 ONI	0.533	0.48	ETHYLENE	ETPM	9	0	S	Best of kind
		0.23	TRANS-2-BUTENE					
	0.551	0.46	ETHYLENE					
		0.23	TRANS-2-BUTENE					
14-Aug-80 ONI	0.470	0.91	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.29	TRANS-2-BUTENE					
	0.466	0.95	ETHYLENE					
		0.32	TRANS-2-BUTENE					
16-Sep-83 ONI	0.228	0.43	ETHYLENE	REAC	5	7	P	Best of kind
		1.57	1-BUTENE					
		1.00	PROPYLENE					
	0.208	0.84	ETHYLENE					
		1.02	1-BUTENE					
		1.04	PROPYLENE					
15-Oct-83 ONI	0.481	1.13	PROPYLENE	REAC	8	5	P	Best of kind
		0.44	ETHYLENE					
		1.60	1-BUTENE					
	0.497	1.00	PROPYLENE					
		0.88	ETHYLENE					
		1.10	1-BUTENE					

Number of runs for this type HC is 9

Table 25. Ethylene Runs, cont.

>>>>> For the HC type of MC Mixture, complex <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
30-Sep-81	ONI	0.300	1.40	UNCMIX	REAC	8	5	L	Best of kind
			0.60	SIMARO					
		0.300	2.00	DODGEMIX II					

Number of runs for this type HC is 1

Total number of runs is 34

Propylene Runs

Table 26.

>>>>>>>>>> For the HC type of 10 Single, olefins <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
20-Jul-77	ONI	0.270	0.65	PROPYLENE	ETPM	8	0	S	Best of kind
		0.280	1.21	PROPYLENE					
12-Oct-77	ONI	0.505	3.56	PROPYLENE	ETPM	4	0	S	Some problems
		0.501	1.72	PROPYLENE					
9-Nov-77	ONI	0.529	3.77	PROPYLENE	ETPM	7	0	S	Satisfactory
		0.537	1.92	PROPYLENE					
10-Jan-78	ONI	0.462	3.25	PROPYLENE	ETPM	8	0	S	Satisfactory
		0.482	4.35	ETHYLENE					
16-Jun-78	ONI	0.634	3.95	ETHYLENE	ETPM	7	0	S	Satisfactory
		0.640	2.00	PROPYLENE					
1-Jul-78	ONI	0.887	1.45	ETHYLENE	ETPM	7	0	S	Best of kind
		0.935	1.51	PROPYLENE					
24-Jul-78	ONI	0.959	2.97	PROPYLENE	ETPM	7	0	S	Satisfactory
		0.952	1.47	PROPYLENE					
30-Jul-78	ONI	0.474	1.32	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.483	1.25	PROPYLENE					
5-Aug-78	ONI	0.248	0.83	PROPYLENE	ETPM	4	0	S	Satisfactory
		0.568	1.55	PROPYLENE					

Table 26. Propylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
6-Aug-78 ONI	0.561	1.69	PROPYLENE	ETPM	4	0	S	Some problems
	0.569	2.59	ETHYLENE					
15-Aug-78 ONI	0.543	1.45	PROPYLENE	ETPM	7	0	S	Best of kind
	0.563	1.58	ETHYLENE					
18-Aug-78 ONI	0.495	0.74	PROPYLENE	ETPM	8	0	S	Best of kind
	0.491	2.88	PROPYLENE					
21-Aug-78 ONI	0.978	1.39	ETHYLENE	ETPM	9	0	S	Satisfactory
	0.981	1.28	PROPYLENE					
18-Oct-78 ONI	0.456	3.12	ETHYLENE	ETPM	9	0	S	Satisfactory
	0.456	1.52	PROPYLENE					
20-Oct-78 ONI	0.460	1.39	PROPYLENE	ETPM	7	0	S	Best of kind
	0.457	3.65	PROPYLENE					
29-Oct-78 ONI	0.498	1.35	PROPYLENE	ETPM	5	0	S	Supporting
	0.495	3.68	PROPYLENE					
2-Nov-78 ONI	0.553	3.52	PROPYLENE	ETPM	8	0	S	Satisfactory
	0.550	1.41	PROPYLENE					
7-Nov-78 ONI	0.441	1.37	PROPYLENE	ETPM	5	0	S	Satisfactory
	0.441	2.67	ETHYLENE					

Table 26. Propylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
31-May-79 ONI	0.491	2.70	PROPYLENE	ETPM	5	0	S	Satisfactory
	0.502	2.69	PROPYLENE					
		50.00	CO					
2-Jun-79 ONI	0.216	1.55	PROPYLENE	ETPM	7	0	S	Best of kind
	0.215	1.56	PROPYLENE					
		40.60	CO					
29-Jul-79 ONI	0.925	1.99	PROPYLENE	ETPM	5	0	S	Satisfactory
	0.928	1.88	PROPYLENE					
		11.98	CO					
13-Aug-79 ONI	0.496	4.39	PROPYLENE	ETPM	7	0	S	Best of kind
	0.188	0.57	PROPYLENE					
24-Jun-81 ONI	0.430	1.58	ISOPRENE	ETPM	8	6	P	Best of kind
	0.433	1.52	PROPYLENE					
29-Aug-82 ONH	0.235		PROPYLENE	ETPM	7	0	N	Supporting
	0.235	1.10	PROPYLENE					
4-Sep-82 ONH	0.220		PROPYLENE	ETPM	9	5	S	Best of kind
	0.231	1.15	PROPYLENE					
10-Sep-82 ONB	0.060		PROPYLENE	ETPM	6	0	N	Supporting
	0.255	1.10	PROPYLENE					

Table 26. Propylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
13-Sep-82 ONB	0.149		PROPYLENE	ETPM	8	3	S	Best of kind
	0.321	1.09	PROPYLENE					
17-Jul-83 ONH	0.267	1.15	PROPYLENE	ETPM	9	5	P	Best of kind
	0.260		PROPYLENE					
21-Jul-83 ONB	0.213	1.15	PROPYLENE	ETPM	9	5	P	Best of kind
	0.000		PROPYLENE					
29-Jul-83 ODI	0.200	1.15	PROPYLENE	ETPM	9	5	P	Best of HC type
	0.198	1.15	PROPYLENE					
31-Jul-83 ONB	0.200	1.15	PROPYLENE	ETPM	9	5	P	Best of kind
	0.000		PROPYLENE					
23-Sep-83 ONI	0.413	1.50	1-BUTENE	REAC	7	6	P	Satisfactory
	0.376	1.50	PROPYLENE					
2-Oct-83 ONI	0.456	3.31	1-BUTENE	ETPM	7	5	L	Satisfactory
	0.430	2.98	PROPYLENE					

Number of runs for this type HC is 33

Table 26. Propylene Runs, cont.

>>>>>>>>>> For the HC type of 1U Single, ole vs ald <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
26-Dec-77	ONI	0.399	2.96	PROPYLENE	ETPM	9	0	S	Satisfactory
		0.407	3.82	ACETALDEHYDE					
27-Feb-78	ONI	0.496	3.95	PROPYLENE	ETPM	7	0	S	Satisfactory
		0.354	1.90	ACETALDEHYDE					
6-Mar-78	ONI	0.511	3.77	PROPYLENE	ETPM	5	0	S	Supporting
		0.374	1.80	ACETALDEHYDE					
31-Mar-78	ONI	0.483	3.82	PROPYLENE	ETPM	6	0	S	Supporting
		0.393	2.00	ACETALDEHYDE					
31-Jul-79	ONI	0.513	1.43	FORMALDEHYDE	ETPM	7	0	S	Supporting
		0.513	5.13	PROPYLENE					
2-Aug-79	ONI	0.205	1.49	PROPYLENE	ETPM	7	0	S	Best of kind
		0.205	1.01	FORMALDEHYDE					

Number of runs for this type HC is 6

Table 26. Propylene Runs, cont.

```
  RUN
  DATE           NOx    HC                           Proj Q I P     GUIDE

>>>>>>>>>>>  For the HC type of   1V  Single, ole vs par   <<<<<<<<<<<

 22-Oct-77 ONI   0.518  3.69   PROPYLENE          ETPM 6 0 S Best of HC type
                 0.525  8.10   N-BUTANE

 24-Oct-77 ONI   0.517  3.69   PROPYLENE          ETPM 5 0 S Satisfactory
                 0.490  8.00   N-BUTANE

Number of runs for this type HC is     2

>>>>>>>>>>>  For the HC type of   1W  Single, ole vs aro   <<<<<<<<<<<

 16-Aug-78 ONI   0.687  1.56   PROPYLENE          ETPM 7 0 S Best of kind
                 0.691  3.93   TOLUENE

Number of runs for this type HC is     1
```

Table 26. Propylene Runs, cont.

>>>>>>>>>>> For the HC type of MB Mixture, simple <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
3-Jun-77	ONI	0.351	1.68	PROPYLENE	ETPM	7	0	S	Best of kind
			0.50	FORMALDEHYDE					
		0.345	1.69	PROPYLENE					
3-Oct-78	ONI	0.497	0.98	ETHYLENE	ETPM	6	0	S	Satisfactory
		0.492	0.14	N-BUTANE					
			1.36	PROPYLENE					
12-Oct-78	ONI	0.479	0.20	ETHYLENE	ETPM	9	0	S	Satisfactory
			1.26	ACETALDEHYDE					
		0.479	1.33	PROPYLENE					
25-Oct-78	ONI	0.444	0.20	ETHYLENE	ETPM	9	0	S	Satisfactory
			1.16	ACETALDEHYDE					
		0.442	1.22	PROPYLENE					
12-Jun-79	ONI	0.500	0.83	PROPYLENE	ETPM	7	0	S	Best of kind
		0.494	0.53	PROPYLENE					
			0.80	ACETALDEHYDE					
13-Jun-79	ONI	0.452	2.81	PROPYLENE	ETPM	7	0	S	Best of kind
		0.443	2.73	PROPYLENE					
			3.16	TOLUENE					

Table 26. Propylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
14-Jun-79 ONI	0.451	1.82	PROPYLENE	ETPM	7	0	S	Best of kind
	0.443	1.79	PROPYLENE					
		3.02	TOLUENE					
16-Aug-79 ONI	0.443	1.42	PROPYLENE	ETPM	9	0	S	Best of kind
	0.436	0.17	ETHYLENE					
		1.30	ACETALDEHYDE					
27-Aug-80 ONI	0.482	2.25	TOLUENE	ETPM	8	0	S	Best of kind
		99.99	CO					
	0.491	1.91	PROPYLENE					
		99.99	CO					
15-Jul-81 ONI	0.300	1.40	N-BUTANE	REAC	7	4	P	Satisfactory
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.60	TOLUENE					
18-Jul-81 TNI	0.300	1.40	N-BUTANE	REAC	8	5	P	Best of kind
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.62	M-XYLENE					

Table 26. Propylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
19-Jul-81 SNI	0.300	1.40	N-BUTANE	ETPM	8	5	P	Best of kind
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.60	M-XYLENE					
22-Sep-81 ONI	0.300	1.40	N-BUTANE	REAC	9	4	L	Satisfactory
		0.60	PROPYLENE					
	0.300	0.42	PROPYLENE					
		0.98	N-BUTANE					
		0.60	TOLUENE					
24-Sep-81 ONI	0.235	1.28	N-BUTANE	REAC	8	5	S	Satisfactory
		0.52	PROPYLENE					
	0.233	0.89	N-BUTANE					
		0.36	PROPYLENE					
		0.77	TOLUENE					
9-Jun-82 ONI	0.290	1.98	N-BUTANE	REAC	7	2	S	Best of kind
		0.64	PROPYLENE					
		0.50	M-XYLENE					
	0.284	1.96	N-BUTANE					
		0.62	PROPYLENE					
		0.53	TOLUENE					
11-Sep-82 ONI	0.500	1.50	PROPYLENE	ETPM	5	6	U	Supporting
		5.00	N-BUTYLNITRATE					
	0.500	1.50	PROPYLENE					
12-Sep-82 ONI	0.692	1.69	PROPYLENE	ETPM	8	6	S	Best of kind
		5.00	N-BUTYLNITRATE					
	0.364	1.69	PROPYLENE					

Table 26. Propylene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
18-Aug-83 ODC	0.280	0.42	PROPYLENE	REAC	7	7	P	Satisfactory
		1.41	N-BUTANE					
		0.79	TOLUENE					
	0.280	0.42	PROPYLENE					
		1.41	N-BUTANE					
		0.79	TOLUENE					
26-Aug-83 ODC	0.310	0.78	TOLUENE	ETPM	9	9	P	Satisfactory
		0.42	PROPYLENE					
		1.40	N-BUTANE					
	0.110		TOLUENE					
			PROPYLENE					
			N-BUTANE					
16-Sep-83 ONI	0.228	0.43	ETHYLENE	REAC	5	7	P	Best of kind
		1.57	1-BUTENE					
		1.00	PROPYLENE					
	0.208	0.84	ETHYLENE					
		1.02	1-BUTENE					
		1.04	PROPYLENE					
15-Oct-83 ONI	0.481	1.13	PROPYLENE	REAC	8	5	P	Best of kind
		0.44	ETHYLENE					
		1.60	1-BUTENE					
	0.497	1.00	PROPYLENE					
		0.88	ETHYLENE					
		1.10	1-BUTENE					

Number of runs for this type HC is 21

Table 26. Propylene Runs, cont.

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of MC Mixture, complex <<<<<<<<<<									
18-Jun-78	ONI	0.354	2.27	N-BUTANE	ETPM	7	0	S	Best of kind
			0.75	PROPYLENE					
		0.354	3.28	UNCMIX					
21-Jun-78	ONI	0.357	1.85	UNCMIX	ETPM	6	0	S	Best of kind
		0.353	1.58	N-BUTANE					
			0.54	PROPYLENE					
3-Sep-81	ONI	0.235	1.78	UNCMIX	REAC	7	4	S	Best of kind
			0.53	SIMARO					
		0.231	1.40	UNCMIX					
			0.46	SIMARO					
			0.57	PROPYLENE					
11-Jul-83	ONI	0.280	1.20	PROPYLENE	REAC	9	5	P	Best of kind
			1.80	SIMMIX2					
		0.265	3.00	SIMMIX2					

Number of runs for this type HC is 4

Table 26. Propylene Runs, cont.

```
   RUN
   DATE           NOx    HC                          Proj Q I P     GUIDE

>>>>>>>>>>  For the HC type of   MV  Mixture, varying       <<<<<<<<<<

 17-Oct-83 ONH    0.493  1.12   PROPYLENE          REAC 9 6 P Satisfactory
                         1.26   TOL/XYL/MIX2
                                ISO-/2,2,4-TM-PE
                                NTANES
                  0.493  1.12   PROPYLENE
                         1.21   TOL/XYL/MIX2
                         2.01   ISO-/2,2,4-TM-PE
                                NTANES

Number of runs for this type HC is      1


>>>>>>>>>>  For the HC type of   S   Single , unclassifed  <<<<<<<<<<

 28-Jan-78 ONI    0.500  3.25    PROPYLENE          ETPM 6 0 S Best of kind
                  0.000

 29-Jan-78 ONI    0.477  3.20    PROPYLENE          ETPM 6 0 S Best of kind
                  0.000

Number of runs for this type HC is      2


Total number of runs is   70
```

N Butane Runs

Table 27.

>>>>>>>>>> For the HC type of 1P Single, paraffins <<<<<<<<<<

RUN DATE		NOx	HC		Proj	Q	I	P	GUIDE
21-Jul-78	ONI	0.243	7.30	N-BUTANE	ETPM	8	0	S	Best of kind
		0.242	15.70	N-BUTANE					
22-Jul-78	ONI	0.548	8.34	N-BUTANE	ETPM	8	0	S	Best of kind
		0.557	17.50	N-BUTANE					
27-Jul-78	ONI	0.266	13.50	N-BUTANE	ETPM	5	0	S	Some problems
		0.509	13.20	N-BUTANE					
24-Aug-78	ONI	0.575	58.00	N-BUTANE	ETPM	9	0	S	Best of kind
		0.803	56.30	N-BUTANE					
25-Aug-78	ONI	0.518	13.20	N-BUTANE	ETPM	7	0	S	Satisfactory
		0.518	26.60	N-BUTANE					
9-Oct-79	ONI	0.207	14.30	N-BUTANE	ETPM	8	0	S	Satisfactory
		0.207	14.20	N-PENTANE					
18-Oct-79	ONI	0.202	15.90	2,3-DIMETHYLBUTANE	ETPM	7	0	S	Satisfactory
		0.201	13.80	N-BUTANE					

Number of runs for this type HC is 7

Table 27. n-Butane Runs, cont.

```
  RUN
  DATE          NOx    HC                          Proj Q I P     GUIDE

>>>>>>>>>>  For the HC type of   1V  Single, ole vs par   <<<<<<<<<<

 22-Oct-77 ONI    0.518  3.69   PROPYLENE          ETPM 6 0 S Best of HC type
                  0.525  8.10   N-BUTANE

 24-Oct-77 ONI    0.517  3.69   PROPYLENE          ETPM 5 0 S Satisfactory
                  0.490  8.00   N-BUTANE

Number of runs for this type HC is     2


>>>>>>>>>>  For the HC type of   1X  Single, other cross   <<<<<<<<<<

 20-Jun-79 ONI    0.187  6.23   N-BUTANE           ETPM 6 0 S Best of kind
                  0.182  6.00   METHYL ETHYL
                                KETONE

Number of runs for this type HC is     1
```

Table 27. n-Butane Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of MB Mixture, simple <<<<<<<<<<								
3-Oct-78 ONI	0.497	0.98	ETHYLENE	ETPM	6	0	S	Satisfactory
	0.492	0.14	N-BUTANE					
		1.36	PROPYLENE					
15-Jul-81 ONI	0.300	1.40	N-BUTANE	REAC	7	4	P	Satisfactory
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.60	TOLUENE					
18-Jul-81 TNI	0.300	1.40	N-BUTANE	REAC	8	5	P	Best of kind
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.62	M-XYLENE					
19-Jul-81 SNI	0.300	1.40	N-BUTANE	ETPM	8	5	P	Best of kind
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.60	M-XYLENE					
22-Sep-81 ONI	0.300	1.40	N-BUTANE	REAC	9	4	L	Satisfactory
		0.60	PROPYLENE					
	0.300	0.42	PROPYLENE					
		0.98	N-BUTANE					
		0.60	TOLUENE					

Table 27. n-Butane Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
24-Sep-81 ONI	0.235	1.28	N-BUTANE	REAC	8	5	S	Satisfactory
		0.52	PROPYLENE					
	0.233	0.89	N-BUTANE					
		0.36	PROPYLENE					
		0.77	TOLUENE					
9-Jun-82 ONI	0.290	1.98	N-BUTANE	REAC	7	2	S	Best of kind
		0.64	PROPYLENE					
		0.50	M-XYLENE					
	0.284	1.96	N-BUTANE					
		0.62	PROPYLENE					
		0.53	TOLUENE					
18-Aug-83 ODC	0.280	0.42	PROPYLENE	REAC	7	7	P	Satisfactory
		1.41	N-BUTANE					
		0.79	TOLUENE					
	0.280	0.42	PROPYLENE					
		1.41	N-BUTANE					
		0.79	TOLUENE					
26-Aug-83 ODC	0.310	0.78	TOLUENE	ETPM	9	9	P	Satisfactory
		0.42	PROPYLENE					
		1.40	N-BUTANE					
	0.110		TOLUENE					
			PROPYLENE					
			N-BUTANE					

Number of runs for this type HC is 9

Table 27. n-Butane Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>> For the HC type of			MC Mixture, complex <<<<<<<<<<					
18-Jun-78 ONI	0.354	2.27	N-BUTANE	ETPM	7	0	S	Best of kind
		0.75	PROPYLENE					
	0.354	3.28	UNCMIX					
21-Jun-78 ONI	0.357	1.85	UNCMIX	ETPM	6	0	S	Best of kind
	0.353	1.58	N-BUTANE					
		0.54	PROPYLENE					
10-Sep-81 ONI	0.235	2.79	UNCMIX	REAC	7	3	S	Best of kind
		0.70	SIMARO					
	0.246	1.02	UNCMIX					
		0.50	SIMARO					
		2.21	N-BUTANE					
12-Sep-81 ONI	0.251	1.68	UNCMIX	REAC	7	4	S	Best of kind
		0.55	SIMARO					
	0.285	1.14	UNCMIX					
		0.39	SIMARO					
		0.62	N-BUTANE					

Number of runs for this type HC is 4

Total number of runs is 23

Toluene Runs

Table 28.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>>>>>>>	Simple Relative Reactivity of Toluene			<<<<<<<<<<<<				
14-Sep-78 ONI	0.292	2.24	TOLUENE	ETPM	5	0	S	Satisfactory
	0.294	0.97	ETHYLENE					
18-Sep-78 ONI	0.503	2.98	ETHYLENE	ETPM	5	0	S	Supporting
	0.496	4.21	TOLUENE					
16-Aug-78 ONI	0.687	1.56	PROPYLENE	ETPM	7	0	S	Best of kind
	0.691	3.93	TOLUENE					
27-Aug-80 ONI	0.482	2.25	TOLUENE	ETPM	8	0	S	Best of kind
		99.99	CO					
	0.491	1.91	PROPYLENE					
		99.99	CO					
>>>>>>>>>>>>>>>	Toluene and its products			<<<<<<<<<<<				
27-Jun-79 ONI	0.337	5.85	BENZALDEHYDE	ETPM	6	0	S	Best of kind
	0.333	15.50	TOLUENE					
11-Aug-80 ONI	0.305	3.18	TOLUENE	ETPM	4	0	S	Best of kind
	0.318	3.14	TOLUENE					
		1.12	BENZALDEHYDE					

Table 28. Toluene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>>>>>>> Toluene addition to propylene <<<<<<<<<<<<								
13-Jun-79 ONI	0.452	2.81	PROPYLENE	ETPM	7	0	S	Best of kind
	0.443	2.73	PROPYLENE					
		3.16	TOLUENE					
14-Jun-79 ONI	0.451	1.82	PROPYLENE	ETPM	7	0	S	Best of kind
	0.443	1.79	PROPYLENE					
		3.02	TOLUENE					
>>>>>>>>>>>>>>> Toluene substitution in Simple Mixture <<<<<<<<<<<<								
15-Jul-81 ONI	0.300	1.40	N-BUTANE	REAC	7	4	P	Satisfactory
		0.60	PROPYLENE					
	0.300	0.98	N-BUTANE					
		0.42	PROPYLENE					
		0.60	TOLUENE					
22-Sep-81 ONI	0.300	1.40	N-BUTANE	REAC	9	4	L	Satisfactory
		0.60	PROPYLENE					
	0.300	0.42	PROPYLENE					
		0.98	N-BUTANE					
		0.60	TOLUENE					
24-Sep-81 ONI	0.235	1.28	N-BUTANE	REAC	8	5	S	Satisfactory
		0.52	PROPYLENE					
	0.233	0.89	N-BUTANE					
		0.36	PROPYLENE					
		0.77	TOLUENE					

Table 28. Toluene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>>>>>> Toluene substitution in complex mixtures <<<<<<<<<<<								
29-Jun-81 ONI	0.200	1.38	UNCMIX	REAC	9	6	P	Best of kind
		0.29	TOLUENE					
	0.200	1.71	UNCMIX					
2-Jun-82 ONI	0.500	1.40	UNCMIX	REAC	7	5	L	Best of kind
		0.36	TOLUENE					
		0.12	M-XYLENE					
	0.500	1.40	UNCMIX					
		0.60	M-XYLENE					
>>>>>>>>>> Relative Reactivity of Toluene / Xylene <<<<<<<<<<								
15-Aug-79 ONI	0.322	4.99	O-XYLENE	ETPM	5	0	S	Satisfactory
	0.320	5.20	TOLUENE					
30-Jul-80 ONI	0.179	3.78	TOLUENE	ETPM	7	0	S	Satisfactory
	0.178	2.23	O-XYLENE					
27-Aug-82 ONI	0.434	1.99	O-XYLENE	ETPM	8	7	S	Supporting
	0.431	3.00	TOLUENE					
27-Oct-82 ONI	0.400	4.50	TOLUENE	ETPM	8	7	S	Satisfactory
	0.399	2.78	O-XYLENE					
1-Aug-83 ONI	0.395	4.59	TOLUENE	ETPM	8	8	P	Best of kind
	0.372	2.62	O-XYLENE					
8-Aug-83 ONI	0.434	6.00	O-XYLENE	ETPM	5	7	L	Satisfactory
	0.421	9.00	TOLUENE					

Table 28. Toluene Runs, cont.

>>>>>>>>>> Relative Reactivity of Toluene / Xylene
in Simple and Complex Mixtures <<<<<<<<<<

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
9-Jun-82 ONI	0.290	1.98	N-BUTANE	REAC	7	2	S	Best of kind
		0.64	PROPYLENE					
		0.50	M-XYLENE					
	0.284	1.96	N-BUTANE					
		0.62	PROPYLENE					
		0.53	TOLUENE					
20-Jul-81 ONI	0.500	1.40	UNCMIX	REAC	6	4	L	Best of kind
		0.60	M-XYLENE					
	0.500	1.40	UNCMIX					
		0.60	TOLUENE					
14-Sep-81 ONI	0.249	1.58	UNCMIX	REAC	8	5	S	Best of kind
		0.61	M-XYLENE					
	0.247	1.65	UNCMIX					
		0.52	TOLUENE					
23-Sep-81 ONI	0.300	1.40	UNCMIX	REAC	8	4	L	Satisfactory
		0.10	ACETALDEHYDE					
		0.50	TOLUENE					
	0.300	1.40	UNCMIX					
		0.10	ACETALDEHYDE					
		0.50	M-XYLENE					

Table 28. Toluene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
29-Sep-81 ONI	0.238	1.95	UNCMIX	REAC	8	5	S	Best of kind
		0.10	ACETALDEHYDE					
		0.53	TOLUENE					
	0.245	1.98	UNCMIX					
		0.10	ACETALDEHYDE					
		0.48	M-XYLENE					
3-Oct-81 ONI	0.300	2.10	UNCMIX	REAC	9	3	L	Best of kind
		0.15	ACETALDEHYDE					
		0.75	M-XYLENE					
	0.300	2.10	UNCMIX					
		0.15	ACETALDEHYDE					
		0.75	TOLUENE					
15-Jul-82 ONI	0.566	1.71	'79 VOLARE AUTO EXHAUST DIRECT	AURE	8	6	S	Best of kind
		0.53	M-XYLENE					
	0.576	1.88	'79 VOLARE AUTO EXHAUST DIRECT					
		0.43	TOLUENE					

Table 28. Toluene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>>>>>> Relative Reactivity of Toluene/ Other Aromatics <<<<<<<<								
8-Jun-82 ONI	0.281	2.25	UNCMIX	REAC	7	6	S	Best of kind
		0.74	ETHYLBENZENE					
	0.281	2.28	UNCMIX					
		0.78	TOLUENE					
6-Jul-82 ONI	0.228	1.43	SIMMIX2	REAC	8	5	S	Best of kind
		0.89	N-PROPYLBENZENE					
	0.225	1.38	SIMMIX2					
		0.84	TOLUENE					
>>>>>>>>>>>>>> Simple Aromatic Compostion Change <<<<<<<<<<<<								
6-Sep-82 ONI	0.456	2.33	TOLUENE	ETPM	9	5	S	Best of kind
		0.54	O-XYLENE					
	0.447	1.90	TOLUENE					
		1.05	O-XYLENE					
7-Sep-82 ONI	0.471	2.48	TOLUENE	ETPM	8	6	S	Best of kind
		0.42	O-XYLENE					
	0.462	2.00	TOLUENE					
		1.02	O-XYLENE					
8-Sep-82 ONI	0.480	3.01	TOLUENE	ETPM	7	7	S	Supporting
		1.70	O-XYLENE					
	0.475	3.80	TOLUENE					
		0.89	O-XYLENE					

Table 28. Toluene Runs, cont.

RUN DATE	NOx	HC		Proj	Q	I	P	GUIDE
>>>>>>>>>>>>>>	Static to Dynamic Series <<<<<<<<<<<							
14-Jun-83 ONB	0.230	1.83	BUTANE/PROPYLENE	ETPM	7	5	P	Best of kind
		0.78	TOLUENE					
	0.000		BUTANE/PROPYLENE					
			TOLUENE					
27-Jun-83 ODC	0.036		BUTANE/PROPYLENE	ETPM	8	5	P	Best of kind
			TOLUENE					
	0.280	1.83	BUTANE/PROPYLENE					
		0.79	TOLUENE					
18-Aug-83 ODC	0.280	0.42	PROPYLENE	REAC	7	7	P	Best of kind
		1.41	N-BUTANE					
		0.79	TOLUENE					
	0.280	0.42	PROPYLENE					
		1.41	N-BUTANE					
		0.79	TOLUENE					
26-Aug-83 ODC	0.310	0.78	TOLUENE	ETPM	9	9	P	Best of kind
		0.42	PROPYLENE					
		1.40	N-BUTANE					
	0.110		TOLUENE					
			PROPYLENE					
			N-BUTANE					

6

Selecting Runs

The purpose of this chapter is to illustrate, using a few examples, how experiments from the UNC Smog Chamber Database might be selected to test mechanisms. After a general discussion, examples of how to select runs to test three different mechanisms will be discussed: an explicit toluene reaction mechanism, a mechanism under dynamic conditions, and an EKMA-type mechanism for urban conditions.

General Selection Guidance

Experiments are not stand-alone entities. No one experiment should ever be modeled alone. Experiments have several unifying characteristics: the matching experiment of the dual run, common seasonal effects, experimental series, chamber characteristics, and common precursor compositions and other conditions.

The dual-experiments were planned so that one side frequently provided a "control," often a more well understood system or one that is used throughout the data set. This side can serve as a reference: *e.g.* the static side of the dynamic series. Experiments conducted side-by-side had the same light and temperature, and usually similar humidity and dilution conditions. The two sides of experiments should be modeled with the same conditions and the same assumptions.

Experiments conducted within a season should all be modeled with similar assumptions of light and chamber characteristics. The modeler should clearly identify any experiments that require unusual conditions relative to other experiments in the season.

Experiments are part of several series. There are series of experiments conducted on different days which are needed to test the mechanism for a single explicit compound. One propylene/NO_x experiment cannot be used to validate propylene chemistry. At a minimum, two experiments such as August 8 and October 22, 1977, are needed to provide a reasonable range of HC-to-NO_x ratios and light and temperature conditions. The same propylene runs could be part of a replicate series where the same conditions were run on the same day in different years to demonstrate reproducibility. This was the case, for propylene/NO_x runs conducted on October 22, 1977 and October 21, 1978. Furthermore, the October 21, 1978 dual-experiment belongs to a series in which humidity effects were studied.

A wide range of experiments were conducted with the same mixtures of precursors. The composition of these mixtures did not vary, and these experiments, therefore, form a series. Models should not treat such mixtures differently in different experiments.

Other recommendations are:

- Follow a hierarchical testing scheme. Model experiments starting at the beginning of hierarchical order with explicitly represented compounds (*e.g.* ethylene for olefin class).
- Model explicit compounds represented in chemical mechanism at a minimum of two HC-to-NO_x ratios.
- Model explicit compounds represented in chemical mechanism in mixtures containing well understood compounds.
- Test model at several compositions of mixtures; test relative ratios of HC classes and specific explicit compounds in mixtures at a minimum of two HC-to-NO_x ratios.
- Model dynamic experiments; follow order discussed below.

Assumptions for Discussion

Some assumptions are necessary for this discussion.

First, it is assumed that modelers have successfully implemented and tested their representation of the diurnal and seasonal effects of solar radiation, chamber air temperature, and chamber absolute humidity. Specific guidance for these items was included in the previous report.[12]

Second, it is assumed that the chamber extraneous processes (*e.g.* background air reactivity, NO_x emissions from chamber walls, and chamber radical sources) that were demonstrated in the chamber characterization runs listed in Table 16, are represented in the mechanism in an acceptable manner and that these are included when modeling chamber runs. Our own modeling of some of the chamber characterization runs suggests that there are at least three chamber related processes that must be considered: emission of NO_x from the chamber walls, emissions of HCHO (or some other radical source) from the walls, and the organic content of the background air used to fill the chamber.[16,17] Models of acetaldehyde/CO characterization experiments suggest that between 0 and 60 ppb of NO_x might have been emitted from the chamber walls in 10 hours. The amount varied depending upon previous runs and degree of chamber venting. The air used to fill the chamber contains, at a minimum, the continental organic background. This background has been described by Whitten and Killus.[18,19] In our modeling studies of the NO_x/CO characterization experiments, we used 35 ppmC of organic background. In addition, 0 to 35 ppb of HCHO might also be emitted from the chamber walls; this amount of HCHO, when combined with the continental background, accounted for the reactivity demonstrated in the NO oxidation runs with and without CO. Modelers should, of course, include background methane and background CO in the initial conditions for their simulations.

Finally, it is assumed that modelers have implemented and tested, with runs listed in Chapters 4 and 5, the chemistry to represent CO, formaldehyde, ethylene, acetaldehyde, propylene, PAN, n-butane, and ketones.

Toluene Mechanism Tests

Let us assume that, as described in Chapter 1, a modeler has constructed an explicit mechanism for toluene based on kinetics data from the literature, for example Atkinson *et al.*[9] and Gery *et al.*,[11] and that they wish to test the representation they have developed. The explicit mechanism for toluene would have to include the reactions for glyoxal, methylglyoxal, benzaldehyde, cresols, nitrotoluenes, and other product species. Some of these reaction products have been tested in the

UNC chambers. Following the suggestions in Chapter 1 concerning the hierarchial development of mechanisms, these parts of the toluene mechanism would be tested first.

Figure 5, for example, shows data from an experiment comparing the reactivity of biacetyl with methylglyoxal. Since benzaldehyde is a major product resulting from $HO^{\cdot}$ attack on the methyl group of toluene, its reactivity is of interest. A run conducted on August 11, 1980 showed that benzaldehyde contributes little to the reactivity of toluene smog reactions. The ability of benzaldehyde versus toluene to oxidize NO to NO_2 was shown in a run conducted on June 27, 1979. The rate of conversion of NO to NO_2 in the benzaldehyde side of this run was not very much faster than that which would be expected from just the background air system.

Clearly not enough toluene reaction product experiments are in the UNC data set for a full hierarchial test. This is, in part, because many of the intermediates are not commercially available or they cannot be synthesized readily for injection into the chamber. Also, many of the species that may form in toluene/NO_x systems have not yet been identified. Carbon balances in smog chambers for toluene and other aromatics are poor. Recent continuous stirred tank reactor experiments with 20-min. resident times have had better carbon yields: ca. 55–75% carbon.[11] This work found a significant amount of methyl-p-benzoquinone, ca. 5%. This, combined with a similar yield for glyoxal and methylglyoxal, suggests that ring cleavage products are not major products. Xylene experiments in the CSTR had higher yields of both the quinones and dicarbonyls. Experiments using quinones are planned in the future.

Table 28 in Chapter 5 listed all experiments in which toluene appeared as a principal reactant. These runs were organized as

- toluene compared to simple olefins,
- toluene mixed with simple olefin compared to simple olefin,
- toluene mixed with its reaction products,
- toluene included in simple mixtures,
- toluene included in complex mixtures,
- toluene compared to other aromatics,
- toluene mixed with xylene,
- toluene in mixtures where the chamber was operated in a dynamic mode.

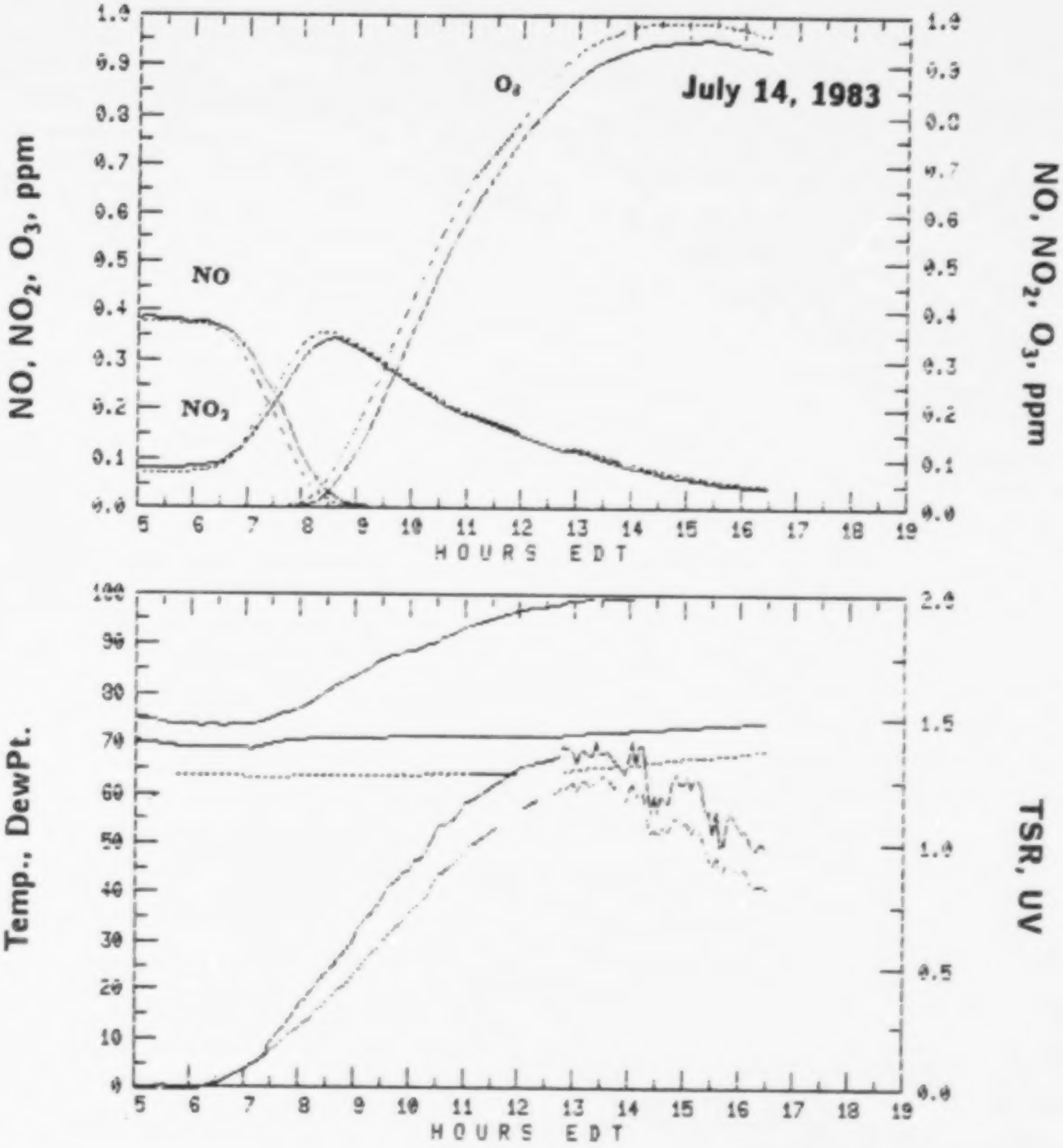

Figure 5. TOP: The behavior of 1.0 ppmC Methylglyoxal and 0.461 ppm NO_x (solid lines) vs 1.0 ppmC of biacetyl and 0.442 ppm NO_x; BOTTOM: Solar radiation and UV time profiles.

The suggestions below follow a three-part strategy: first model toluene in simple systems, then model toluene in increasingly complex mixtures, then model toluene in comparison to other aromatics.

Toluene in Simple Systems

We suggest that when first modeling toluene, the model developer should test against toluene/NO_x experiments that were run side-by-side with either propylene/NO_x or ethylene/NO_x systems. Many insights have been developed in modeling these simple olefin systems. All of the unique features associated with a particular day in terms of light, temperature, NO_x, O_3, HCHO, and PAN measurements, will be evident in modeling the ethylene or propylene side of these dual runs. Hence, a modeler can save substantial time in fitting these runs first rather than "tuning" the toluene chemistry to fit a unique but perhaps anomalous feature of a given day. Experiments which involve toluene/NO_x versus ethylene/NO_x or propylene/NO_x are listed in Table 28.

To assure that the radical sources in the toluene mechanism are well understood, it is useful to model experiments where the radical cycling was modified without introducing another photolytic source of radicals. Such experiments have been conducted by adding a high concentration of CO to one side of the chamber. When a high CO level was added to one side of a match propylene/NO_x run (June 2, 1979 for example), the side with added CO made slightly more O_3. Further, in this case, a matched propylene/NO_x run was conducted on June 1, 1979 and the NO_x and O_3 profiles were perfectly matched. The presence of high CO in one side of the June 2 propylene run reduced the loss of NO_2 by successfully competing with NO_2 for $HO^\cdot$. Since the reaction of $HO^\cdot$ with NO_2 results in a loss of photolyzable nitrogen, the side without CO lost nitrogen from the smog system at a faster rate and thus formed less O_3. The Aug. 27, 1980 run in which ca. 50 ppm CO was added to each side of a run with toluene/NO_x on one side and propylene/NO_x on the other is an example of this process. A correct model will be able to account for the effect of the added CO.

Hydrocarbon/NO_x systems involving toluene have a potential to remove nitrogen through unique pathways not found in simple olefin systems. An interesting experiment, which was essentially the opposite of the CO addition experiment of June 2, 1979, was an experiment in which a high concentration of toluene was added to a matched propylene experiment. Normally, adding more HC would result in more or at least the same O_3. In this case, however, the potential nitrogen loss caused by the toluene might offset any additional reactivity contributed by the extra HC. As described in Chapter 1, this behavior was predicted by Whitten and Killus using a model for toluene. It is illustrated in the June 14, 1979 run shown in Figure 2 in Chapter 1. Clearly a correct toluene mechanism must be able to reproduce this nitrogen loss process.

Toluene in Mixtures

The simplest mixture to approximate urban conditions would be a proplyene/butane/toluene mixture. Such a mixture would also provide a test of toluene chemistry. One example is the September 24, 1981 run listed in Table 28. In this substitution run, toluene carbon was substituted for propylene/butane carbon and the reactivities of the substituted and un-substituted mixtures were compared. The proplyene-to-butane carbon ratio was 3-to-7 on both sides and toluene was substituted for 40% of the total carbon. The NO_x and O_3 profiles for this runs are shown in Figure 6. The substitution of toluene into this simple mixture ***did not significantly alter*** the NO_x or O_3 behavior on the substituted side. Unlike toluene, substituting o-xylene into such a system significantly increases the reactivity of the substituted side, as we will discuss in the following section.

A similar experiment, but substituting toluene into the more complex 11 component paraffin/olefin UNCMIX resulted in a similar outcome as in the propylene/butane experiment, *e.g.* essentially matched reactivity (see June 29, 1981 in Table 28). Further experiments using toluene in mixtures will be described below.

Models must correctly represent the reactivity contribution of aromatics to urban mixtures; toluene is a significant species in the aromatic class.

Toluene Compared with Other Aromatics

The relative reactivities of toluene and o-xylene are illustrated in Figures 7 and 8, which show data for the August 1, 1983 run. These figures show that o-xylene, with almost half the initial carbon, was much more reactive than toluene. Although the rate of $HO^{\cdot}$ attack on toluene (9,400 $ppm^{-1}min^{-1}$) is approximately half that of $HO^{\cdot}$ and o-xylene, the much higher reactivity of o-xylene is also caused by its reaction products. According to Gery,[20] toluene and $HO^{\cdot}$ reactions produce glyoxal and methylglyoxal in almost equal molar yields. Glyoxal is not as reactive as methylglyoxal. $HO^{\cdot}$ attack on o-xylene, on the other hand, produces primarily methylglyoxal

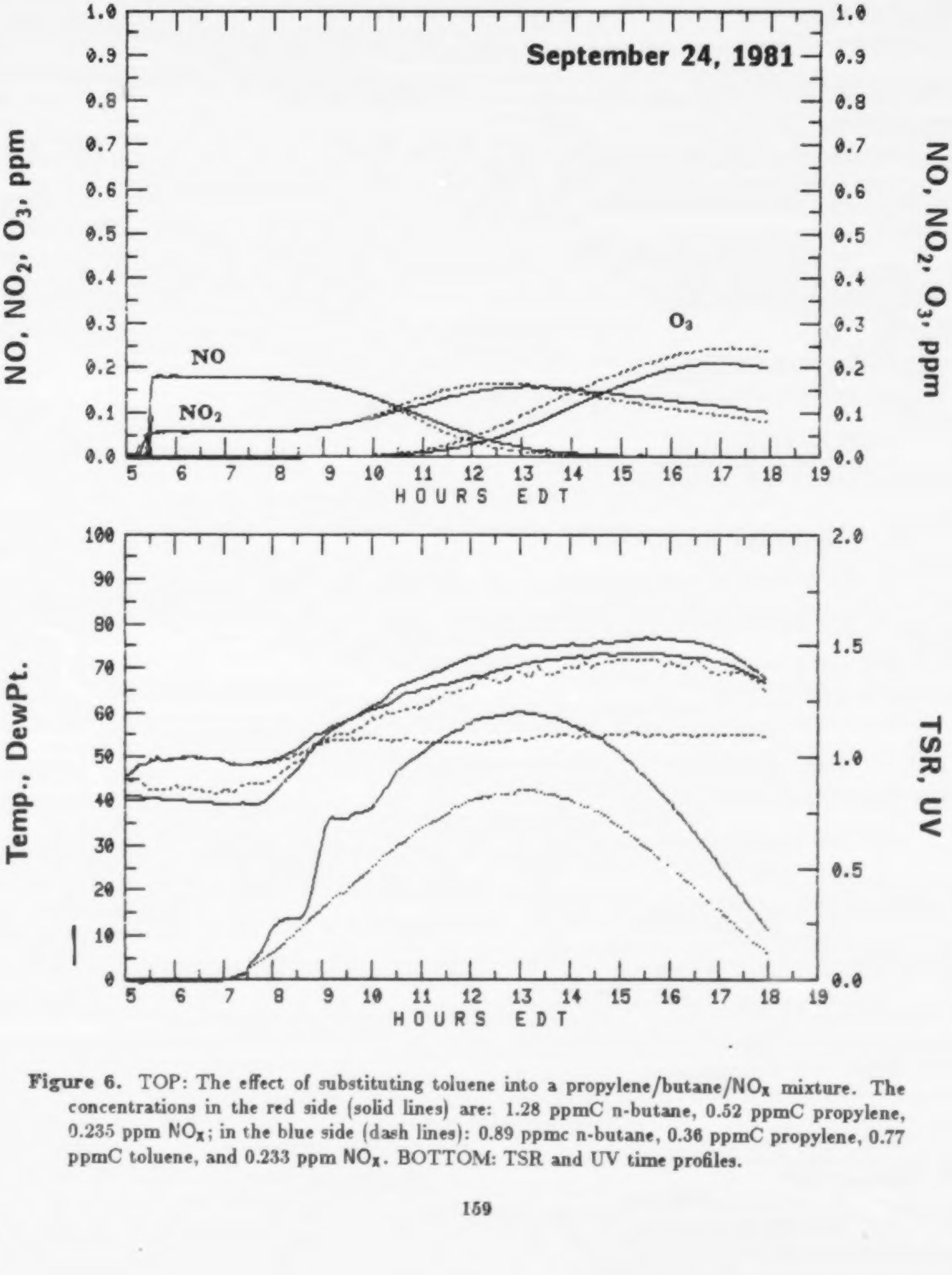

Figure 6. TOP: The effect of substituting toluene into a propylene/butane/NO_x mixture. The concentrations in the red side (solid lines) are: 1.28 ppmC n-butane, 0.52 ppmC propylene, 0.235 ppm NO_x; in the blue side (dash lines): 0.89 ppmc n-butane, 0.36 ppmC propylene, 0.77 ppmC toluene, and 0.233 ppm NO_x. BOTTOM: TSR and UV time profiles.

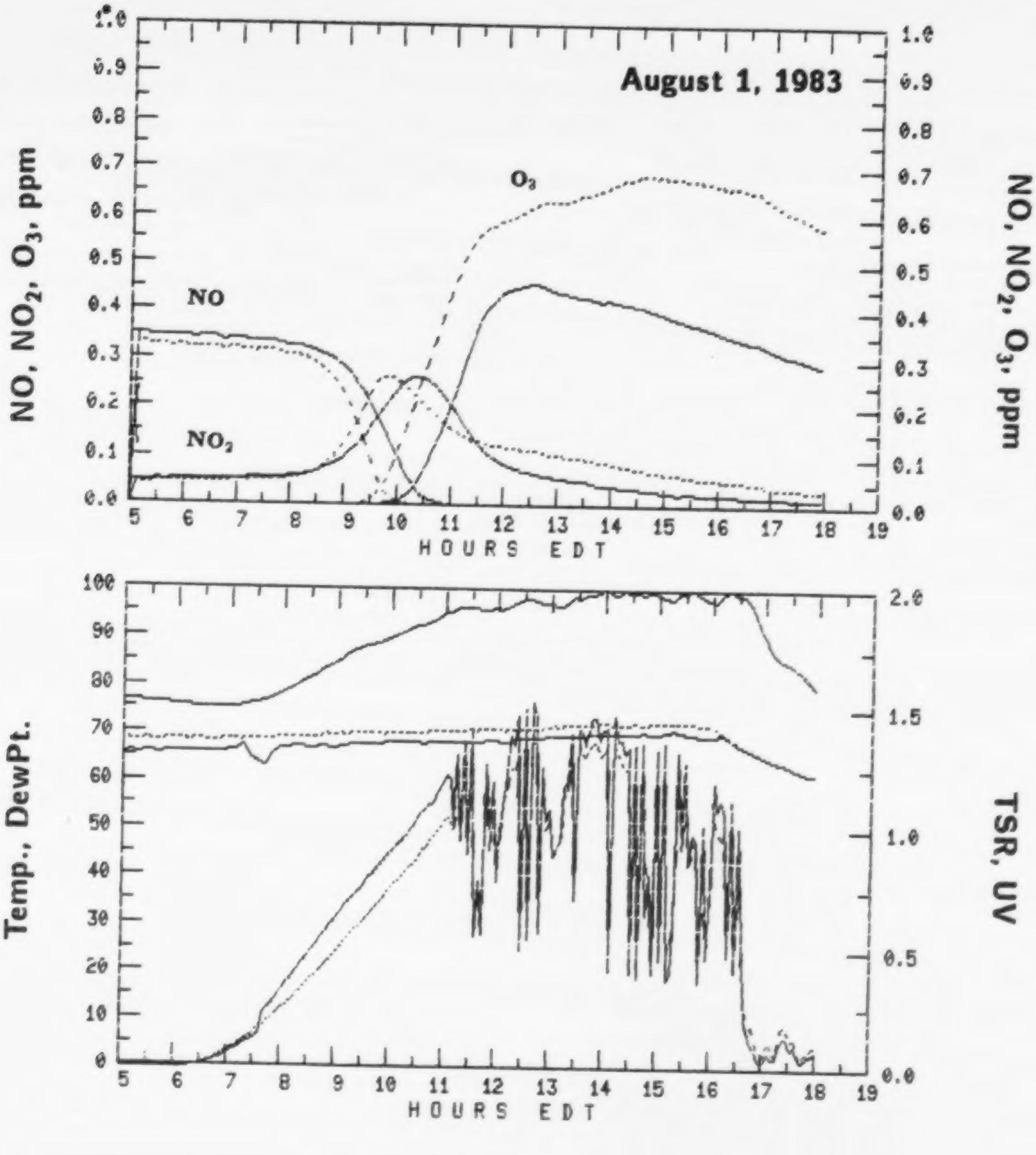

Figure 7. TOP: Toluene/NO$_X$ vs o-Xylene/NO$_X$. The concentrations in the red side (solid lines) are: 4.59 ppmC toluene and 0.395 ppm NO$_X$: in the blue side (dash lines), 2.62 ppmC o-xylene,and 0.372 ppm NO$_X$. BOTTOM: TSR and UV time profiles.

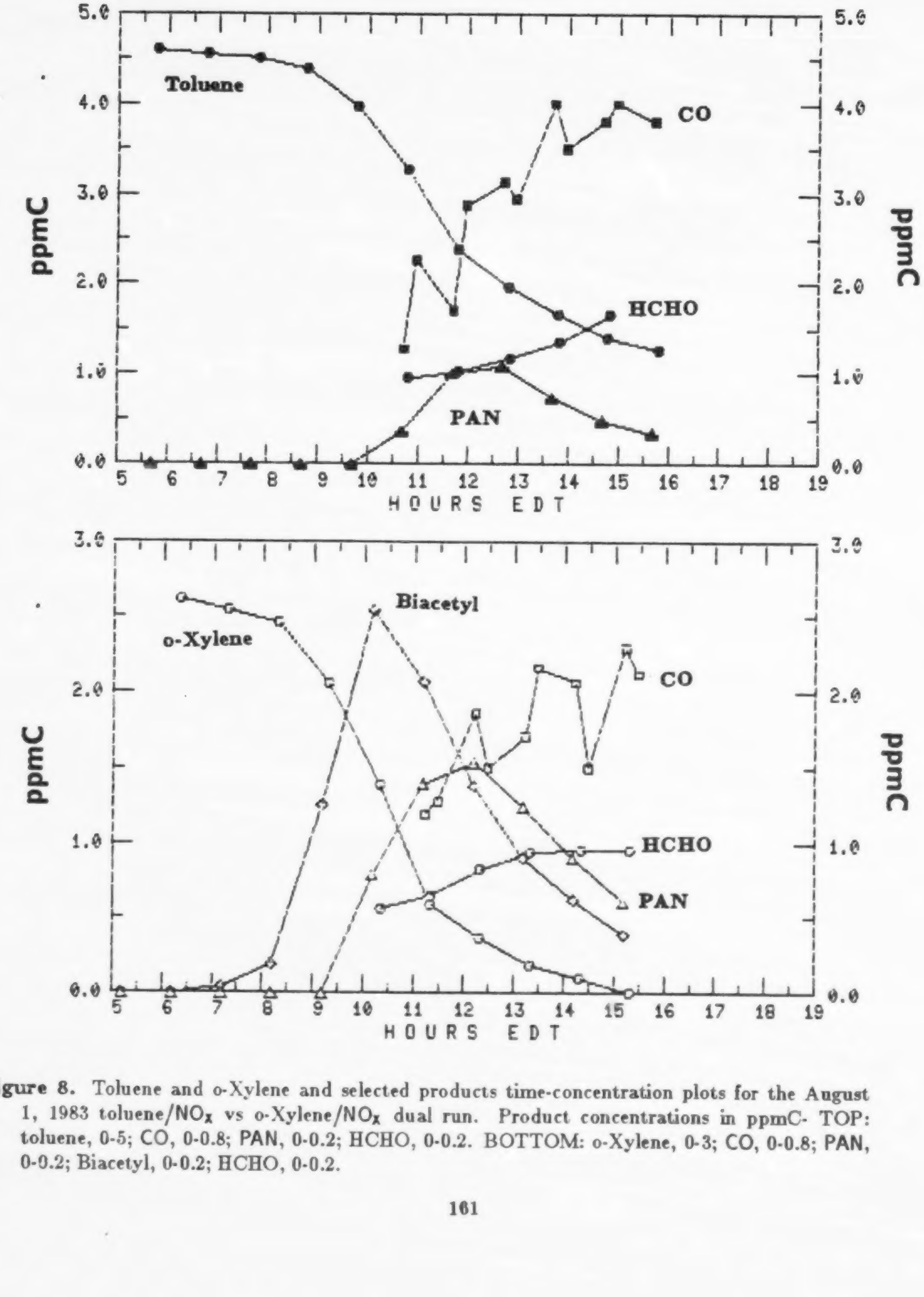

Figure 8. Toluene and o-Xylene and selected products time-concentration plots for the August 1, 1983 toluene/NO_x vs o-Xylene/NO_x dual run. Product concentrations in ppmC- TOP: toluene, 0-5; CO, 0-0.8; PAN, 0-0.2; HCHO, 0-0.2. BOTTOM: o-Xylene, 0-3; CO, 0-0.8; PAN, 0-0.2; Biacetyl, 0-0.2; HCHO, 0-0.2.

and biacetyl, and the dicarbonyl carbon yields are approximately three times those in toluene/$HO^{\cdot}$ systems. Both of these product compounds are very reactive and readily react to produce NO to NO_2 oxidizing radicals and carbonyl compounds that photolyze to make new radicals. The ability to model both sides of this experiment would indicate a good understanding of the dependence of reactivity upon aromatic structure.

The next level of testing involves the use of simple mixtures of toluene and o-xylene with different concentrations. Three runs of this type were conducted on September 6, 7, and 8, 1982. These runs were planned so that the ratios of toluene to o-xylene were different on the two sides of the chamber. A model which fits one side must fit th[illegible]her at the same time. September 6 and 7 were both very high quality runs. Th[illegible]y conditions on September 8, 1982 were somewhat overcast. Sept. 6 is plotted in Figure 9.

The comparison of toluene and xylene was also carried out in mixtures. These experiments are listed in Table 28. In the June 9, 1982 experiment, shown in Figure 10, each aromatic (toluene and m- xylene, in this case) was present at ca. 20% of the total carbon in a 1-to-3 propylene/butane mixture on the two sides. In the September 14, 1981 experiment, shown in Figure 11, each aromatic was present at ca. 25% of the total carbon in the UNCMIX. Xylene's greater reactivity is quite evident even at these levels.

Toluene was also compared with other aromatics besides o-xylene and m-xylene. For example, Figure 12 compares the reactivity of toluene with ethyl-benzene in the UNCMIX. Table 28 lists other relative comparisons that would allow a bridge to be formed between a validated toluene mechanism and other aromatics.

Other Toluene Test Runs

Toluene was not only used in the experiments listed in Table 28, it was a significant component in many of the mixtures listed in Tables 10 and 11. Many of these will be discussed in sections below.

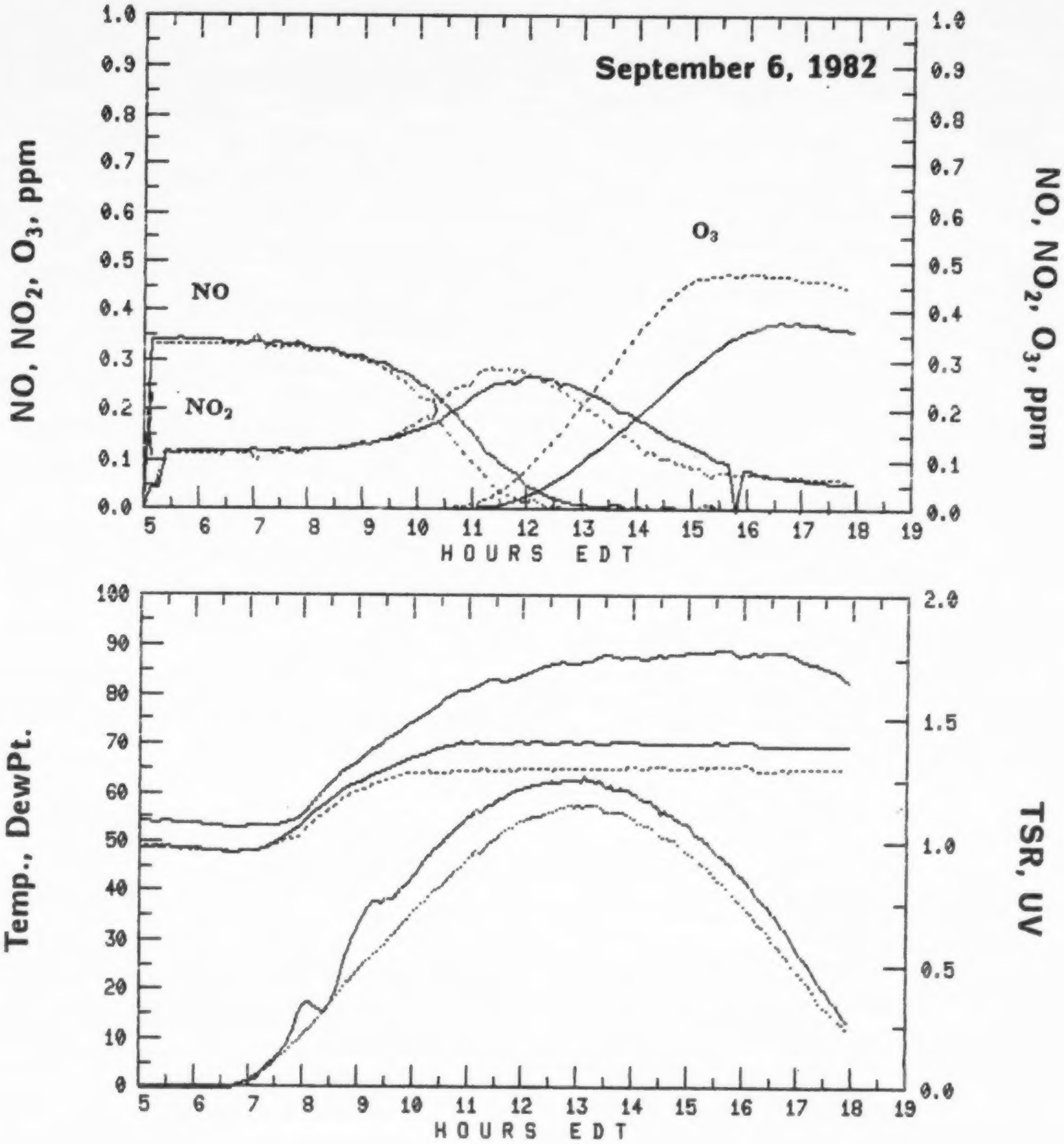

Figure 9. TOP: The effect of different toluene/o-Xylene ratios on smog systems. The concentrations in the red side (solid lines) are: 2.33 ppmC toluene, 0.54 ppmC o-Xylene, and 0.456 ppm NO_x. In the blue side (dash lines): 1.90 ppmC toluene, 1.05 ppmC o-Xylene and 0.447 ppm NO_x. BOTTOM: TSR and UV time profiles.

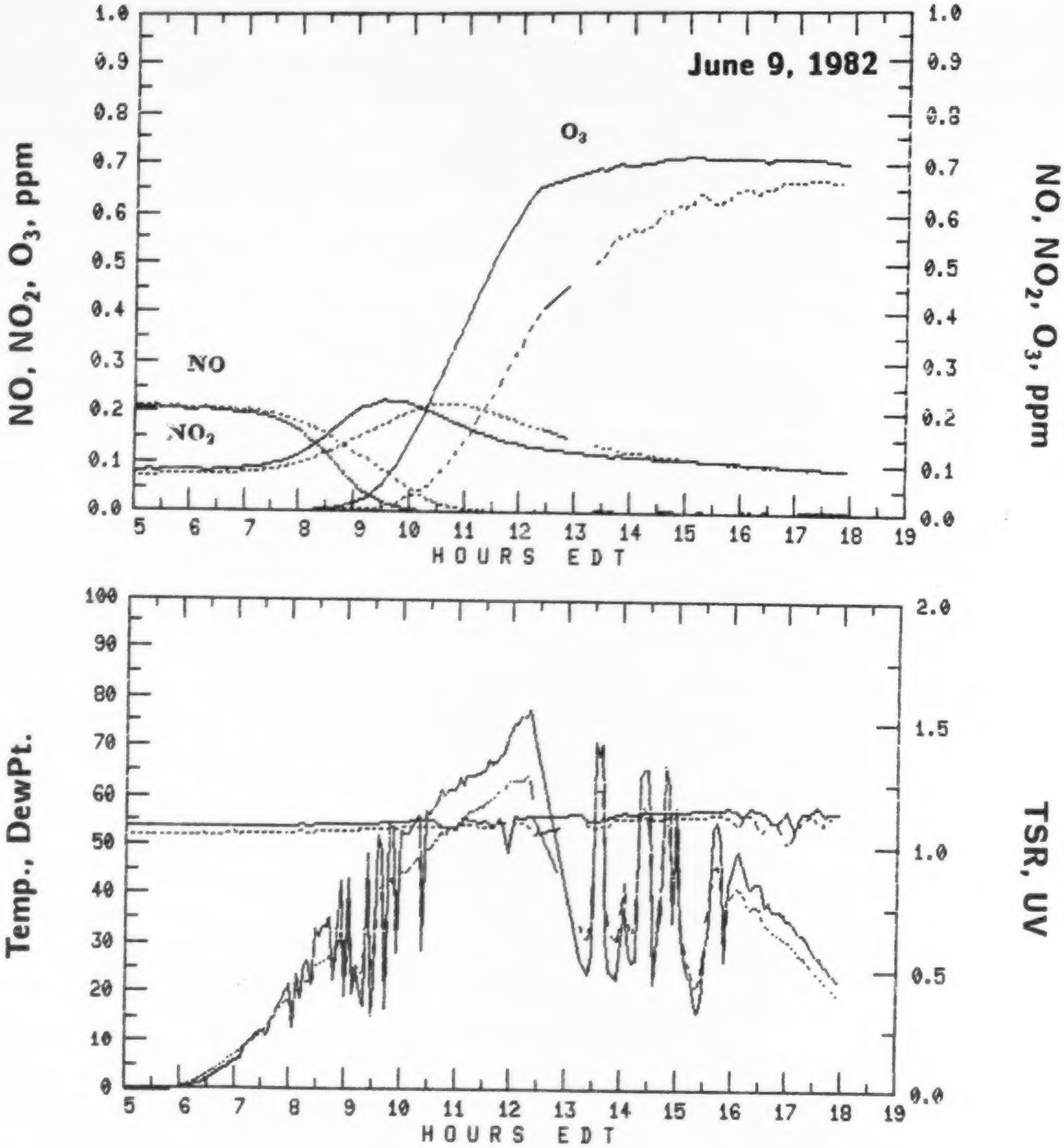

Figure 10. TOP: The effect of substituting either toluene or m-xylene into a propylene/butane mixture. The concentrations in the red side (solid lines) are: 1.98 ppmC n-butane, 0.64 ppmC propylene, 0.50 ppmC m-xylene, and 0.290 ppm NO_x; in the blue side (dash lines), 1.96 ppmC n-butane, 0.62 ppmC propylene, 0.53 ppmC toluene and 0.284 ppm NO_x. BOTTOM: TSR and UV time profiles.

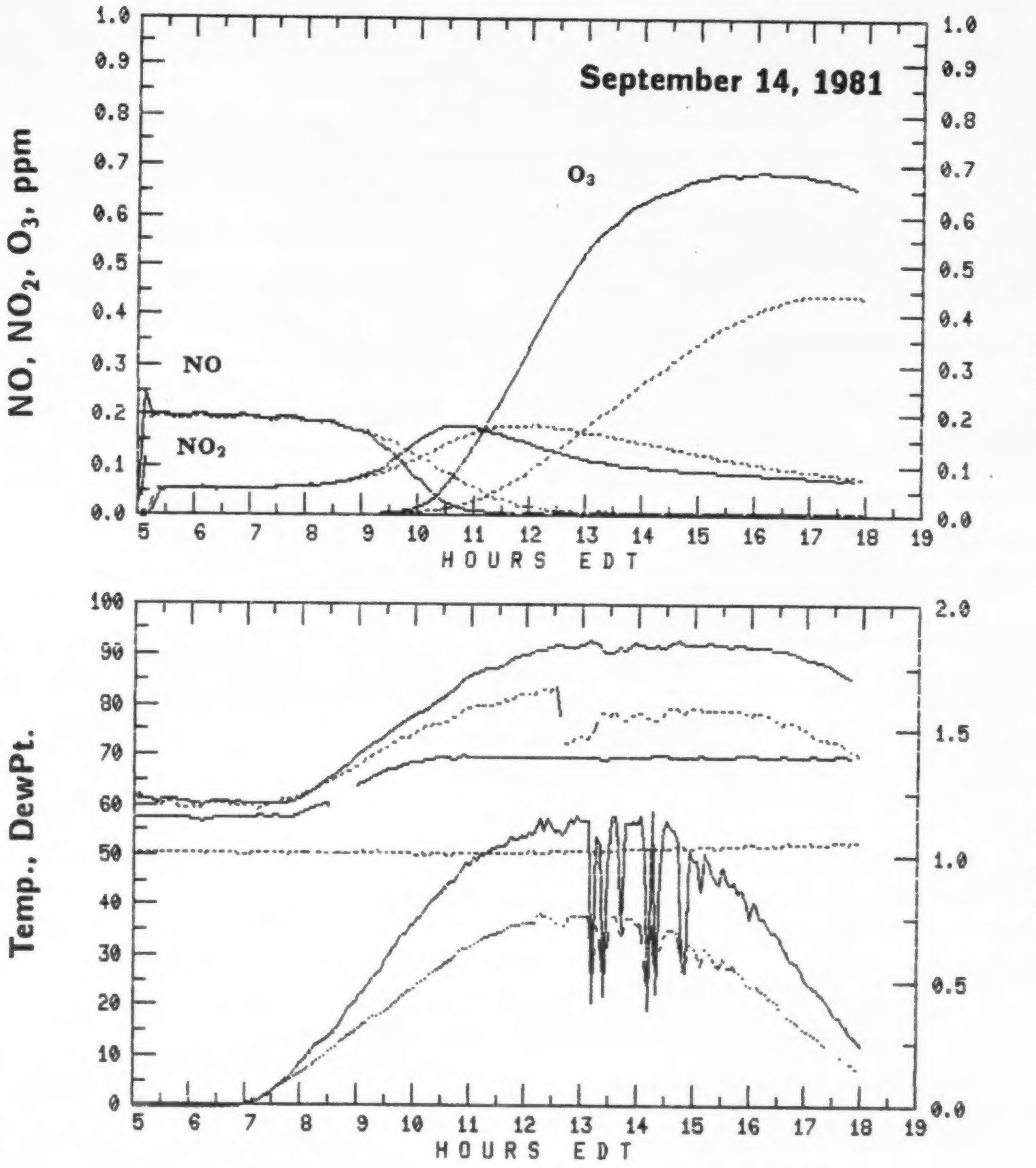

Figure 11. TOP: The effect of substituting either toluene or m-xylene in the UNC mix. The concentrations in the red side (solid lines) are: 1.58 ppmC UNC mix, 0.61 ppmC m-xylene, 0.249 ppm NO_x; in the blue side (dash lines) 1.65 ppmC UNC mix, 0.52 ppmC toluene and 0.247 ppm NO_x. BOTTOM: TSR and UV time profiles.

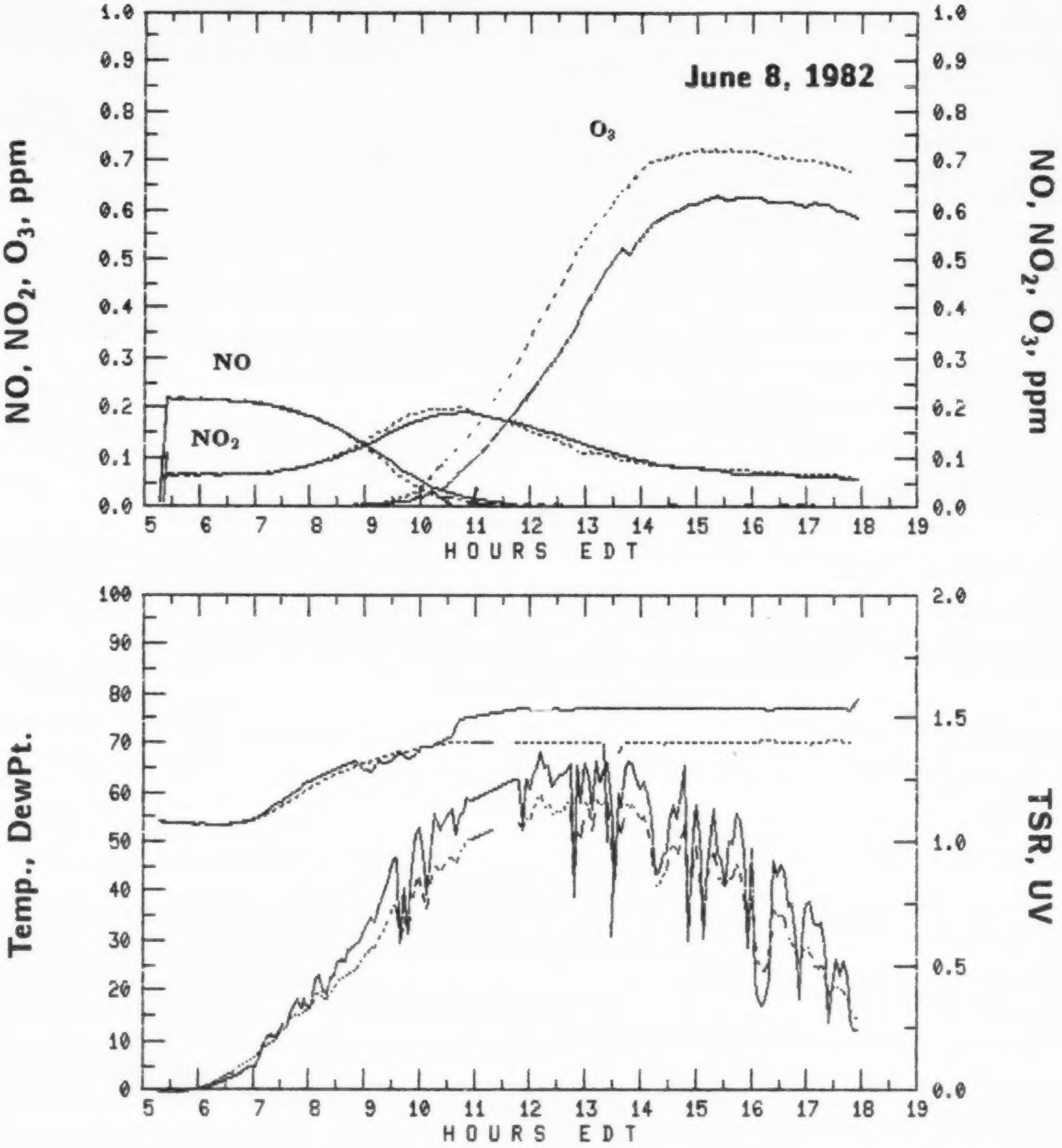

Figure 12. TOP: The effect of substituting either toluene or ethylbenzene into the UNC mix. The concentrations in the red side (solid lines) are: 2.25 ppmC UNC mix, 0.74 ppmC ethylbenzene, 0.281 ppm NO_x; in the blue side (dash lines) 2.28 ppmC UNC mix, 0.78 ppmC toluene and 0.281 ppm NO_x. BOTTOM: TSR and UV time profiles.

Dynamic Condition Tests

The dynamic experiments conducted at UNC investigated the effects of three major processes:

- large dilution rates,
- continuous injection of O_3 precursors,
- varying precursor composition.

All three of these processes are active in the atmosphere and chemical mechanisms should be tested with experiments in which all three processes are important. As in the hierarchical approach for modeling complex precursor mixtures, experiments are needed which test each of the effects separately. This increases the probability of detecting possible compensating errors or misrepresentations which might yield fortuitous modeling results. To clearly demonstrate the operating condition effects, simple HC systems were used initially. Furthermore, in line with the hierarchical approach, tests of more complex systems were performed with or against more familiar, and presumably, better understood systems. These simpler systems serve as a reference for the individual model test.

Successful modeling of the experiments conducted to test the effects of each major dynamic process individually is a natural prerequisite to successfully modeling the more realistic experiments in which all major dynamic processes were investigated. The dynamic experiments conducted at UNC are not a complete test for chemical mechanisms (they are far simpler than conditions of the atmosphere), however, any chemical mechanism designed to model the atmosphere certainly should be able to model these experiments.

Because propylene/NO_x chemistry is well understood, the initial experiments were conducted with propylene as the sole HC. Further, similar concentrations of NO_x and propylene were used in the initial experiments at each level of increasing complexity to provide an easy transition between the various combinations of processes (*e.g.* no dilution, dilution, initial injection only, continuous injection). More complex experiments followed the propylene-only ones, sometimes involving dynamic processes on both sides of the chamber to demonstrate the relative effects of the processes. Table 29 briefly describes the experiments and lists the experiments in the order in which they should probably be modeled.

Table 29. Recommended Order For Modeling Of Dynamic Experiments

1) Large Dilution; All Injections Initially; Dilution Tracers
    - ▹ Propylene
        - ○ 29-Jul-1983
    - ▹ Complex mixture (alkane, olefin, aromatic)
        - ○ 6-Oct-1983
2) No Dilution; Continuous Injection; Injection Tracers
    - ▹ Propylene injected continuously; NO_x injected initially
        - ○ 4-Sep-1982
        - ○ 17-Jul-1983
    - ▹ No Dilution; Complex mixture (alkane, olefin, aromatic) injected continuously on both sides with one side receiving 50% HCof the other; NO_x injected initially on both sides.
        - ○ 12-Sep-1983
    - ▹ No Dilution; Propylene and NO_x injected continuously.
        - ○ 13-Sep-1982
        - ○ 21-Jul-1983
        - ○ 31-Jul-1983
    - ▹ No Dilution; Propylene/butane/toluene and NO_x injected continuously.
        - ○ 14-Jun-1983
3) Large Dilution; Continuous Injection: Dilution and Injection Tracers
    - ▹ Propylene/butane/toluene/NO_2 injected initially; O_3 injected continuously.
        - ○ 18-Aug-1983
    - ▹ Propylene/butane/toluene/NO_x injected continuously;
        - ○ 27-Jun-1983
    - ▹ Propylene/butane/toluene/NO_x/O_3 injected continuously;
        - ○ 26-Aug-1983

Table 29 continued

4) No Dilution; Continuous Injection of HC in both sides; Varying HC Composition; five and six component HC mixtures; final concentration and composition would have been the same on both sides if there were no reactions of the HC.

- ▷ NO_x injected initially on both sides;
  - Each side had initial NMHC that was the same concentration but different species.
  - Each side had continuously injected HC that were the same concentration (ppmC) but different species.
  - Concentration of NMHC injected into chamber was the same at any time but the composition was different.
    - ○ 9-Jul-1983
- ▷ NO_x injected initially on one side and continuous on the other; other conditions were a repeat of the 9-Jul-1983 experiment
  - ○ 22-Aug-1983
- ▷ NO_x injected initially on both sides;
  - Each side had initial NMHC that were different concentrations and different species.
  - Each side had continuously injected HC that were different concentration (ppmC) and different species.
  - Concentrations and composition of NMHC injected into chamber were different at any time.
    - ○ 17-Oct-1983

Dilution Only Experiments

The effects of dilution have not been carefully studied. It is known that the effect is non-linear with respect to precursors and O_3 production.[21] That is, since O_3 is in dynamic equilibrium with NO and NO_2, diluting the precursors by a factor of five does not necessarily reduce the $[O_3]$ by a factor of five. Until now, few smog chamber experiments investigating this subject had been conducted.

Several dilution experiments were conducted with a constant dilution rate resulting in ca. five-fold dilution. Dilution experiments also were conducted at several levels of complexity including single HC species, simple HC mixtures, complex HC mixtures. These experiments also investigated O_3 added to the dilution air. In all dilution experiments, inert tracers were added initially to both sides of the chamber. These tracers were used to quantify the actual dilution rates.

Two simple dilution experiments were conducted with no continuous injections of NO_x and HC, *i.e.* otherwise standard static chamber conditions. These experiments must be modeled before attempting to model the more complex experiments. The simplest experiment (July 29, 1983) was conducted with a propylene and NO_x system. In this experiment, two identical amounts of NO_x and propylene were injected into each side before sunrise; one side was then diluted by a factor of five over the course of the run (see Figure 13). The second experiment (October 6 1983) was conducted with a 16 component HC mixture and NO_x. In this experiment two different dilution rates were compared using an otherwise matched HC/NO_x system.

Continuous Injection

These experiments were designed to allow a hierarchical approach to testing continuous injection without the influence of other major dynamic processes. Experiments were conducted with continuous injections of HC only, HC and NO (with and without background O_3 present), and HC and NO_2. The HC reactants ranged from propylene to complex mixtures.

To provide a highly reproducible injection method for the continuous injection, continuously stirred tank reactor (CSTR) systems were constructed from 1- to 50-liter glass vessels. In use, the CSTRs were purged with N_2, the total amount of reactant mass was injected into the vessel at the beginning of the experiment, and N_2 carrier gas was supplied to the inlet of the CSTR. The outlet of the CSTR went to the chamber injection manifold. In this manner, the initial contents of the CSTR

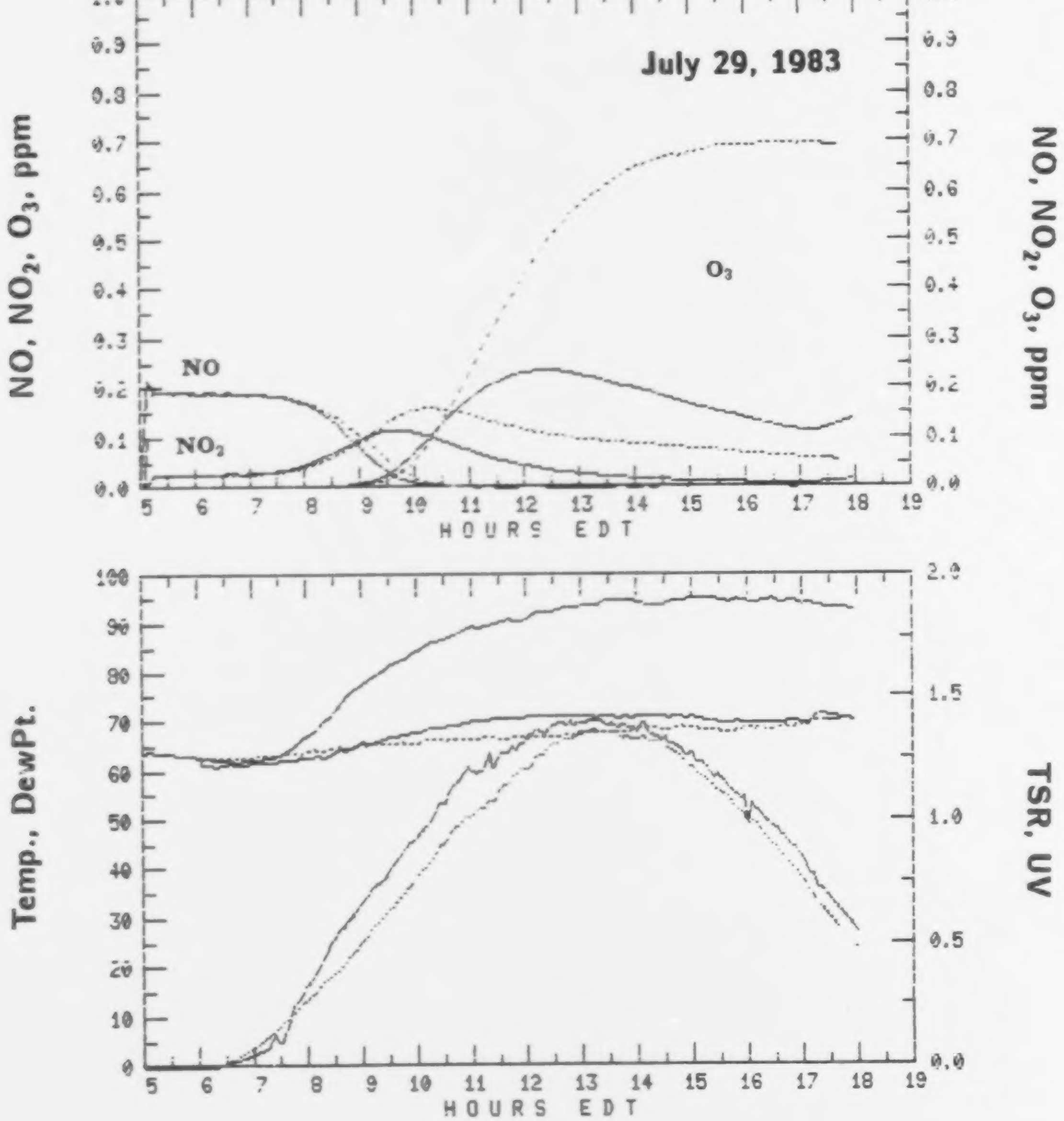

Figure 13. TOP: Static Injections of 1.1 ppmC propylene 0.22 ppm NO_x (Solid Line) vs Static Injections of 1.1 ppmC propylene 0.22 ppm NO_x (Dashed Line). Red side diluted. BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation.

were exponentially injected into the chamber. In addition, tracers were added to the CSTRs so that each injection could be carefully quantified; these CSTR tracers were different from the dilution tracers added initially to the chambers. The volumes of the vessels, the flowrates, and the masses of reactants used were also precisely determined. Further details on the experimental conditions are given by Sexton.[22]

Three experiments were conducted in which only HC was injected continuously. Of these, two experiments were of the simplest type, in which only propylene was continuously injected throughout the experiment; all the NO_x was injected initially (*i.e.* before sunrise). One experiment was conducted in cool fall conditions (September 4, 1982) and the other in warm summer conditions (July 17, 1983). On both days, a matching experiment with no dilution was conducted in the other side of the chamber. A correct model should be able to predict both sides of both experiments; this would demonstrate not only an adequate description of the continuous injection process, but also a correct representation of the effects of seasonal temperature and light changes.

The other continuous HC injection experiment used a complex HC mixture that was injected continuously on both chamber sides (September 12, 1983). In this experiment, matched initial NO_x conditions were established in both chamber sides before dawn. Continuous injections of HC (using the same composition for both sides) started at dawn. Each side also used the same injection-time profile. The difference between the two sides was that the injection rate on one side was half the injection rate of the other side. This experiment might be considered a simple "EKMA" test which examines the effects of a 50% reduction in HC emissions over a city (see Figure 14). Both sides should be modeled with the same chamber characteristic assumptions, light, temperature, humidity, and HC composition.

The next level of complexity introduces continuous injections of NO_x, as well as, the HC. These more complex experiments were designed to be compared with the two HC-only continuous injection experiments described above: September 4, 1982 and July 17, 1983. Three experiments were conducted with propylene as the sole HC. In the experiment conducted on September 13, 1982, the object was to perform a normal "static" run on one side of the chamber (*i.e.* all reactants injected before sunrise) and to perform a "dynamic" injection run on the other side of the chamber (*i.e.* all reactants continuous injected over 10 hours). The amounts of material injected into the "dynamic" side were equivalent to those initially injected into the "static" side. The July 21, 1983 experiment is similar to the September 13, 1982

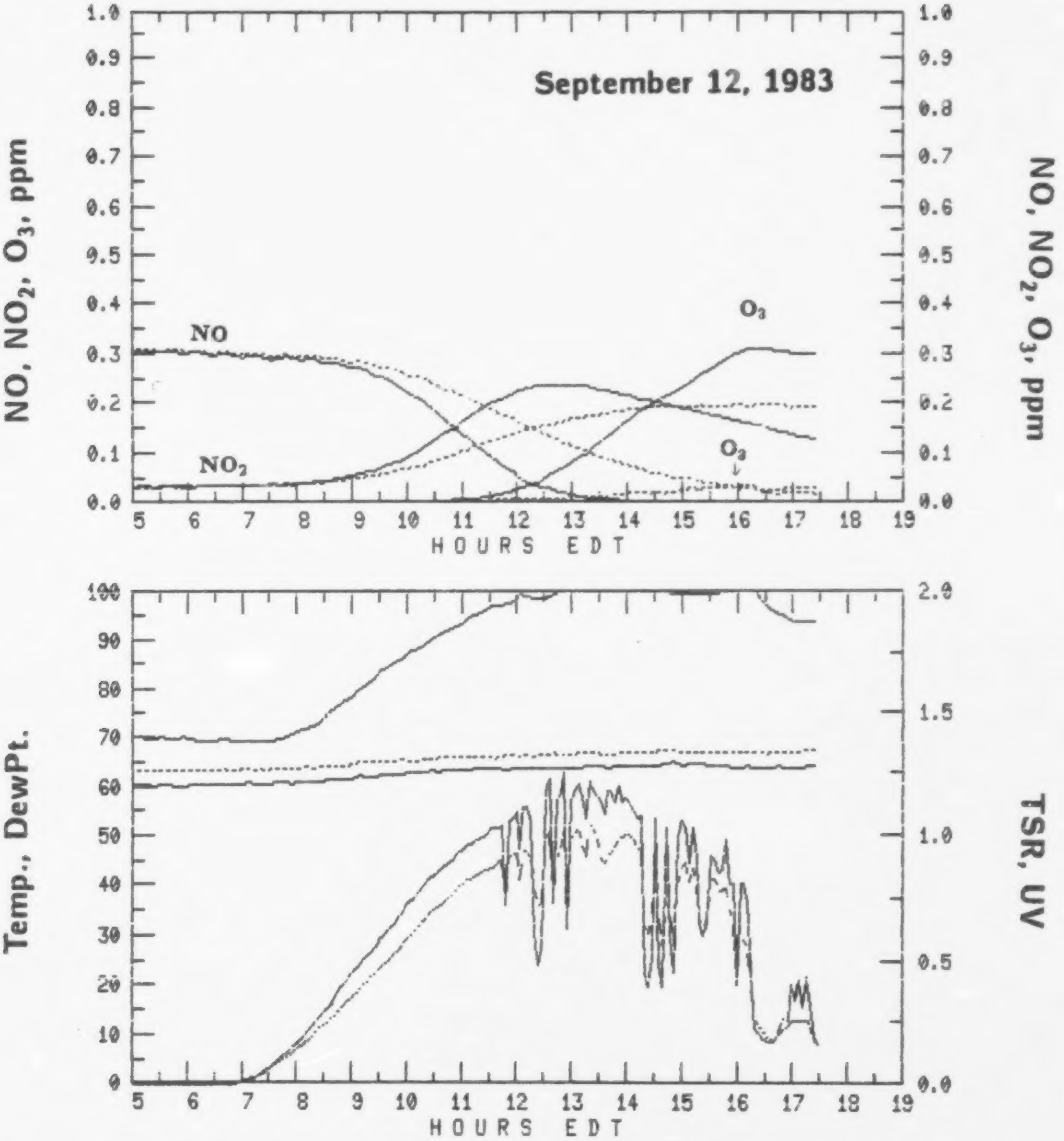

Figure 14. TOP: Static 0.5 ppmC UNC mix, 0.335 ppm NO_x with CSTR Injection of 0.2 ppmC toluene, 0.3 ppmC isopentane, 0.25 ppmC 2,2,4-trimethylpentane, 0.05 ppmC of m-xylene and o-Xylene (Dashed Line) vs Static 1.0 ppmC UNC mix, 0.335 ppm NO_x with CSTR Injection of 0.4 ppmC toluene and 0.6 ppmC isopentane, 0.5 ppmC 2,2,4-trimethylpentane, 0.1 ppmC m-xylene and o-Xylene (Solid Line). BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation.

experiment except that a background concentration of 0.05 ppm of O_3 was present initially on both sides. In the "static" side, this initial O_3 is titrated with the initial NO; in the "dynamic" side, the NO concentration is always low, increasing the possibility of O_3 reacting with the olefins in the injected HC. The July 31, 1983 experiment is similar to the September 13, 1982 experiment except that the NO_x injected was all NO_2 and no initial O_3 was present. These three experiments provide similar, familiar systems but with different conditions which should effect the relative importance of different mechanistic pathways.

The next level of complexity for continuous injection experiments was to use a simple hydrocarbon mixture that represents the three major classes of hydrocarbons: propylene, butane, toluene. The experiment was conducted on June 14, 1983. The conditions for this experiment—one side "static", the other side "dynamic"—were similar to the experiment conducted on September 13, 1982, providing a bridge between only propylene and mixtures. The profiles for this important experiment are shown in Figure 15. The "static" side of this experiment has been modeled with both the ALW and CB3 mechanisms and the results have been subjected to extensive analysis; both models fit both sides well.[7,22]

Dilution and Continuous Injection

These experiments are the next most complex; they combine the dilution processes tested in the first group of experiments above (*e.g.* July 29, 1983) with the continuous injection processes in the second group (*e.g.* June 14 and July 31, 1983). All experiments were conducted with the propylene, butane, toluene, and NO_x precursor mixture used in the June 14, 1983 experiment. Thus there is a transition bridge between the simpler continuous-injection-only experiments and the more complex dilution-and-injection experiments. Each experiment in this set was conducted with a reference static experiment. The "dynamic" sides of these experiments must be modeled concurrently with their matching "static" counterparts.

A frequent feature of large dilution in atmospheric simulations is the entrainment of O_3 into the reacting mixture as the mixing height changes; the O_3 comes from the air that was above the mixing height. To simulate this process in the UNC dynamic experiments, we used an O_3 generator to inject O_3 into the return manifold while the chamber was being diluted with outside air. Sometimes the outside air also contained small amounts of O_3; these were monitored with a separate O_3 monitor.

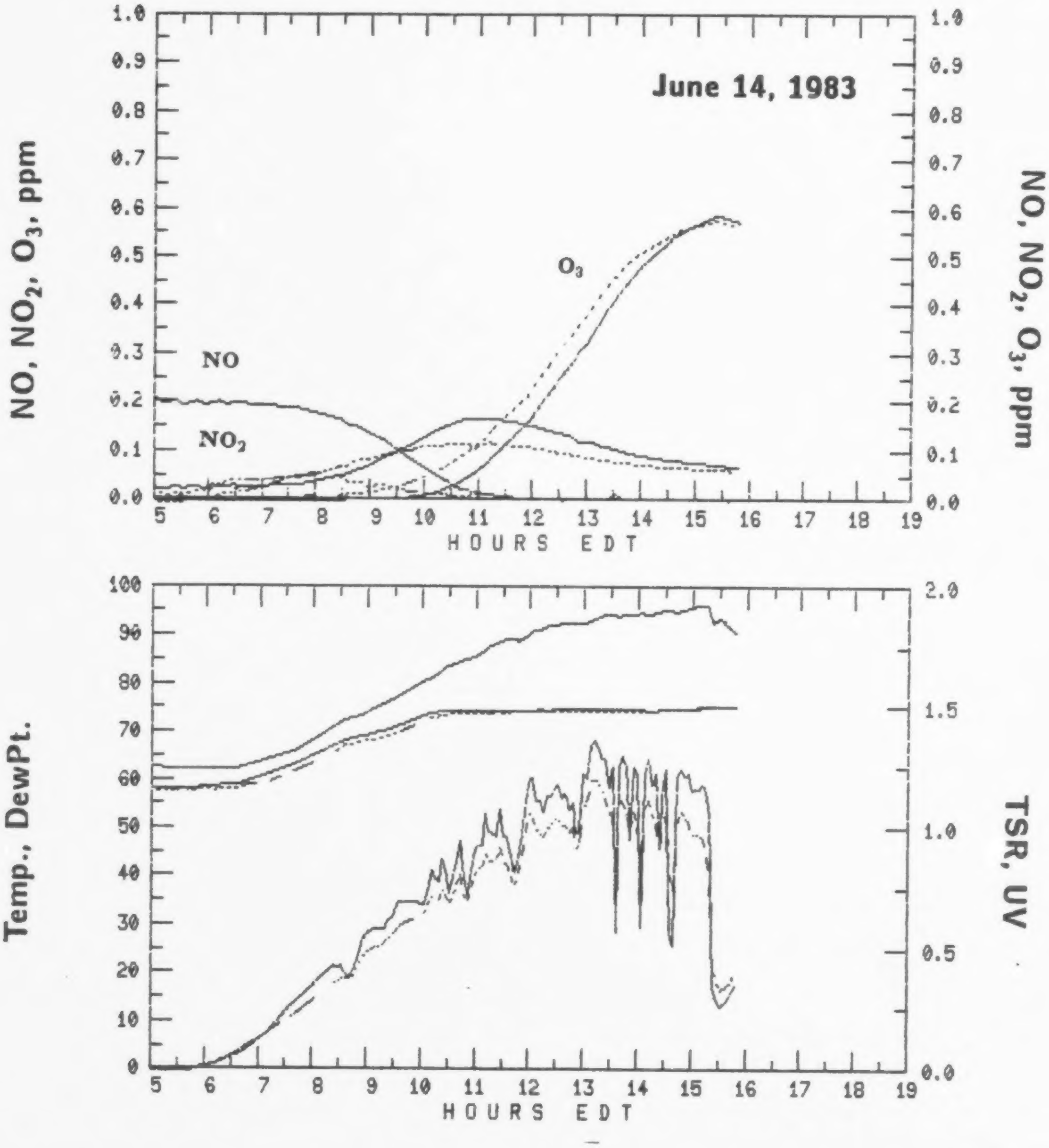

Figure 15. TOP: Static Injections of 0.44 ppmC propylene, 1.31 ppmC butane, 0.84 ppmC toluene 0.22 ppm NO$_X$ (Solid Line) vs Continuous CSTR Injection of 0.44 ppmC propylene, 1.31 ppmC butane, 0.84 ppmC toluene and 0.22 ppm NO$_X$ (Dashed Line). BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation.

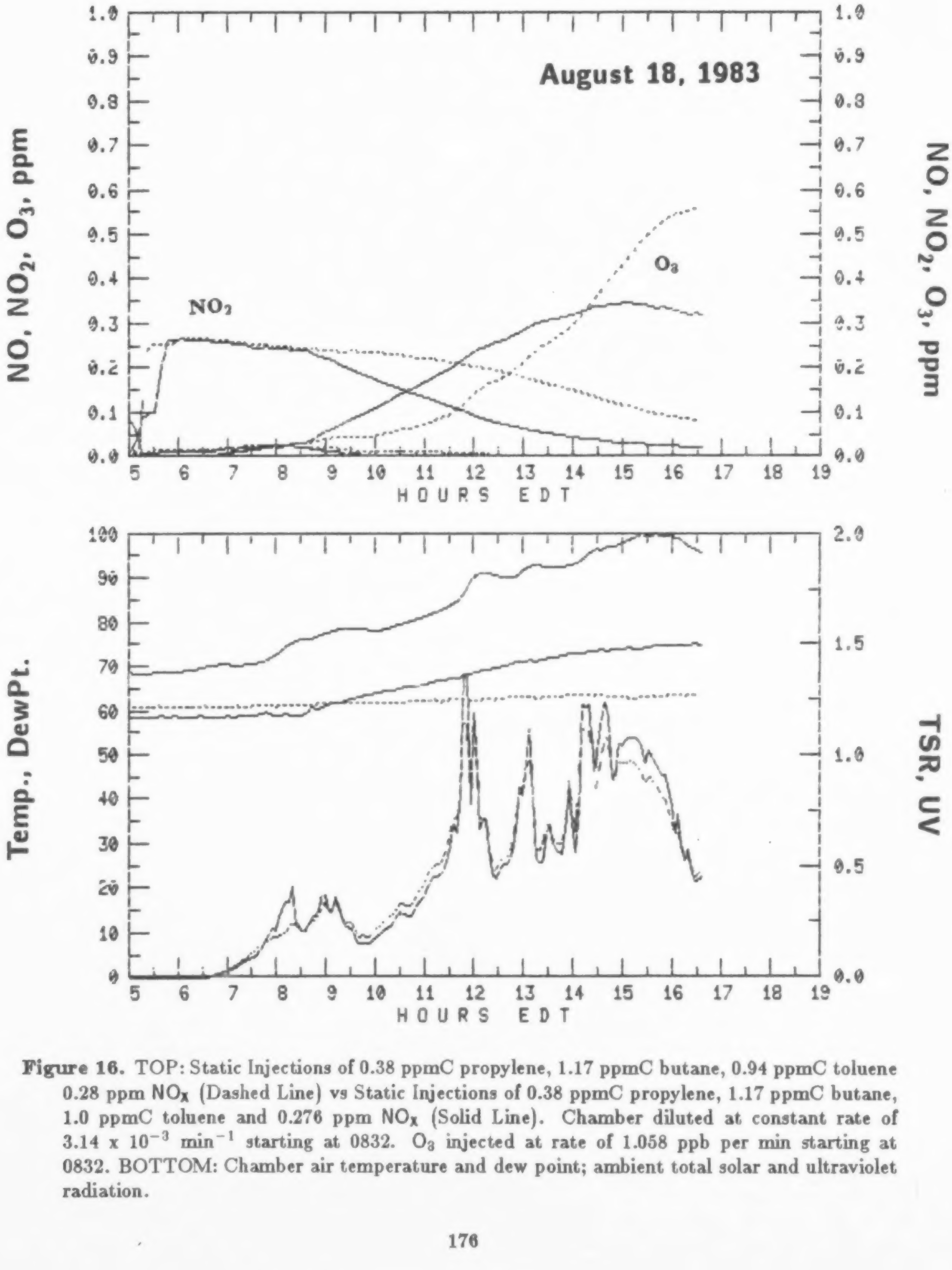

Figure 16. TOP: Static Injections of 0.38 ppmC propylene, 1.17 ppmC butane, 0.94 ppmC toluene 0.28 ppm NO$_x$ (Dashed Line) vs Static Injections of 0.38 ppmC propylene, 1.17 ppmC butane, 1.0 ppmC toluene and 0.276 ppm NO$_x$ (Solid Line). Chamber diluted at constant rate of 3.14 x 10^{-3} min^{-1} starting at 0832. O$_3$ injected at rate of 1.058 ppb per min starting at 0832. BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation.

To assure that models would correctly account for entrained O_3, an experiment that tested only the effect of continuously injection O_3 while diluting the chamber was performed. In the experiment of August 18, 1983 (see Figure 16) both sides of the chamber had matched initial concentrations of the propylene, butane, toluene mixture and NO_x. Because O_3 was to be injected continuously on one side, all the NO_x was injected as NO_2 on both sides to minimize the reaction between NO and O_3 on the "dynamic" side. One side was diluted (like the June 29, 1983 and October 6, 1983 experiments described above) at a constant rate and O_3 was injected at a constant rate to mimic the entrainment process. Although the solar radiation conditions for the run are not ideal, we feel that the general trends in this experiment must be successfully modeled before proceeding to the next, more complex, experiments.

Two experiments were conducted in which both dilution and continuous injections were used.

The June 27, 1983 experiment (Figure 17) was similar to the June 14, 1983 experiment: continuous injections of HC and NO_x but, in addition, the chamber contents were diluted. This is a key experiment in testing models for dynamic processes and both sides must be modeled successfully.

The August 26, 1983 (Figure 18)experiment was similar to the June 27, 1983 experiment except that a large amount of O_3 was directly injected with the HC and NO_x while the chamber contents were also being diluted.

Varying HC Composition

The experiments discussed above were conducted with one of the assumptions inherent in many EKMA models: the composition of the HC precursor emissions is constant throughout the day. In the urban atmosphere, however, emissions vary constantly giving rise to a varying composition of the total HC. To test this process, several experiments were conducted using simple HC mixtures of five to six compounds and with at least one species in each major HC class.

These experiments involved no dilution (other than the normal 1% per hour) and *both* sides of the chamber used:

- initially injected NO_x that matched on the two sides;
- initially injected HC;
- continuously injected HC.

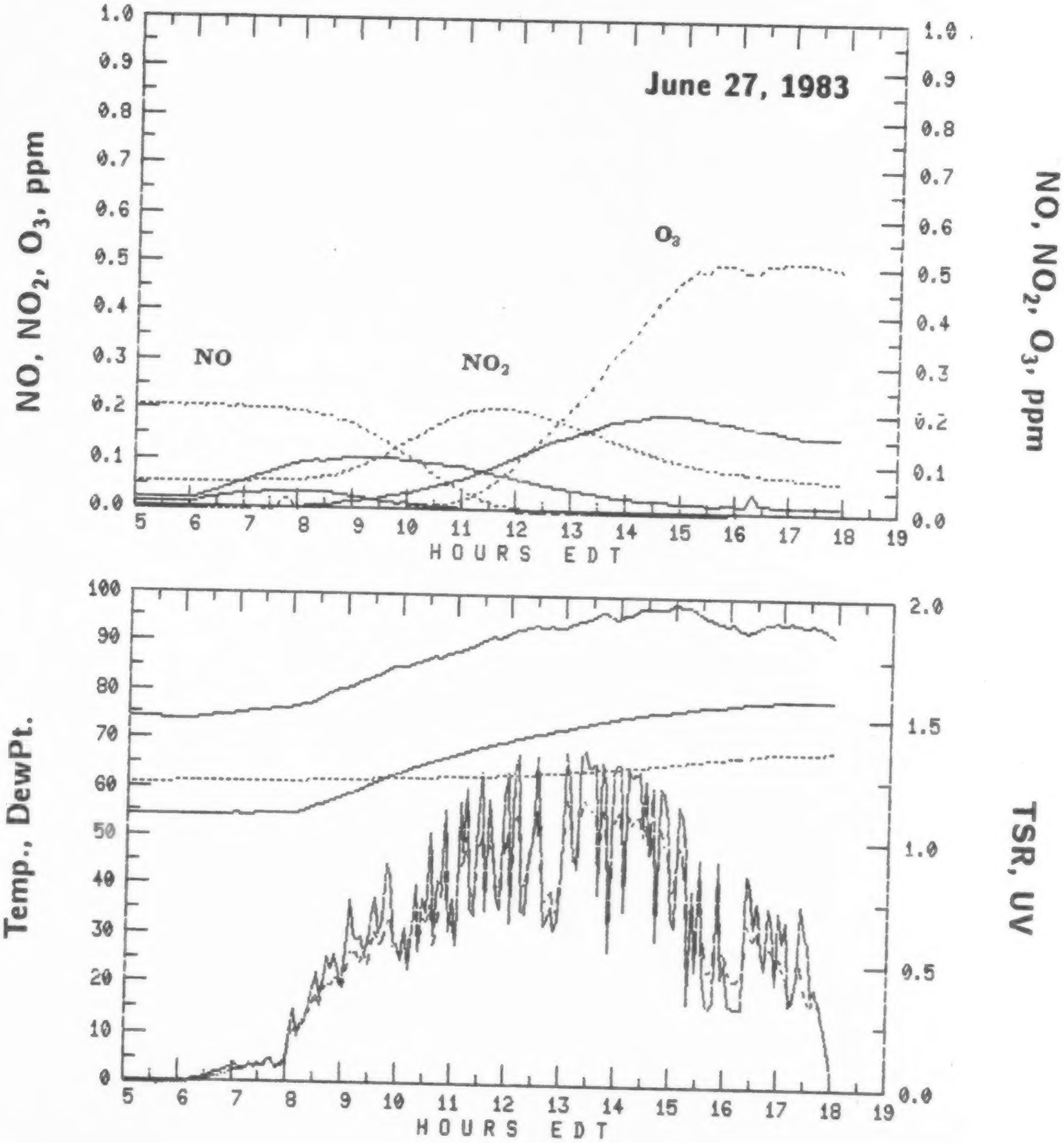

Figure 17. TOP: Static Injections of 0.47 ppmC propylene, 1.47 ppmC butane, 0.94 ppmC toluene 0.22 ppm NO$_x$ (Dashed Line) vs Continuous CSTR Injection of 0.44 ppmC propylene, 1.31 ppmC butane, 0.84 ppmC toluene and 0.22 ppm NO$_x$ (Solid Line). Chamber diluted at constant rate of 3.15 x 10^{-3} min^{-1} starting at 0800. BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation.

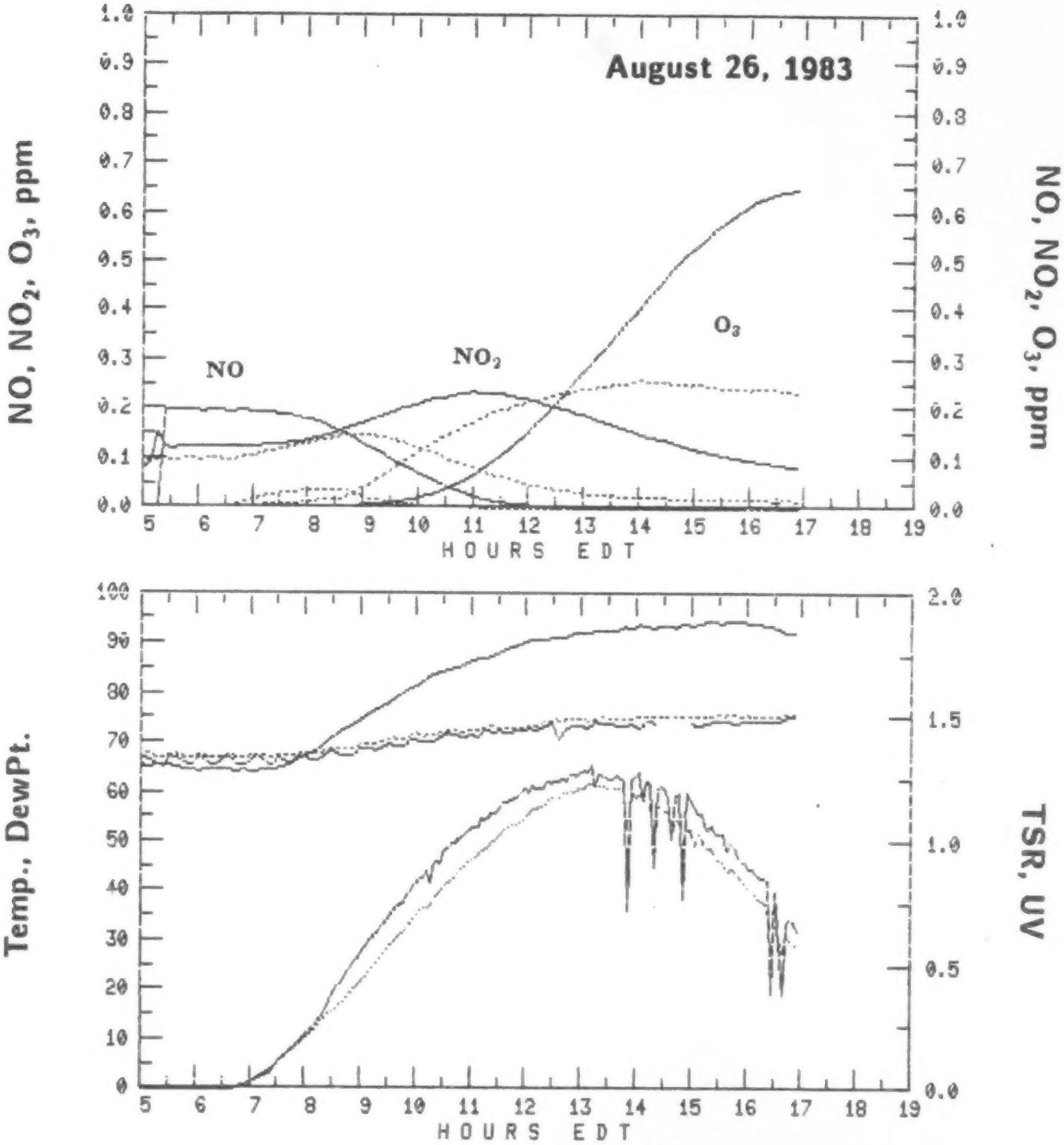

Figure 18. TOP: Static Injections of 0.49 ppmC, propylene, 1.29 ppmC butane, 0.84 ppmC toluene and 0.22 ppm NO$_x$ (Solid Line) vs Continuous CSTR Injection of 0.44 ppmC propylene, 1.31 ppmC butane, 0.84 ppmC toluene and 0.22 ppm NO$_x$ (Dashed Line). Chamber diluted at constant rate of 3.69 x 10^{-3} min^{-1} starting at 0837. O$_3$ injected at rate of 1.338 ppb per min starting at 0837. BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation.

In addition, if no HC had reacted, the two sides of the chamber would both have had the same *final* concentration and composition of HC after 10 hours of continuous injection in all runs of this type.

In the experiment conducted on July 9, 1983, the two sides of the chamber had the same initial NMHC concentration, but differed in the NMHC composition. That is, different species were used to achieve the same initial NMHC on the two sides. Likewise, different species were continuously injected which, if no reaction had occurred during the experiment, would have produced the same final NMHC concentration in each side, as well as, the same final NMHC composition. This experiment used two olefins, two alkanes, and two aromatics as the HC mixture. Five species (two olefins, two alkanes, and one aromatic) were injected initially in each side; the other aromatic was injected continuously and it was different for the two sides. On one side, toluene was injected continuously while m-xylene was injected initially; one the other side, m-xylene was injected continuously while toluene was injected initially. At any time during the run, if no reaction had occurred, the total aromatic concentration would have been the same on both sides. Many regular EKMA models would utilize an average aromatic composition. Modeling of both sides of this experiment will provide a dramatic test for these EKMA models.

The experiment conducted on October 17, 1983 (Figure 19) also used varying HC composition similar to July 9. In this experiment, however, the initial NMHC concentrations and composition on the two sides were different (as opposed to the same on July 9). Likewise, the continuously injected NMHC was different in both concentration and composition. One one side, 1.1 ppmC propylene was continuously injected and on the other side, 1.0 ppmC isopentane and 1.0 ppmC 2,2,4-trimethylpentane were continuously injected. Thus, on one side, 1.1 ppmC of HC and on the other side 2.0 ppmC of HC were injected over 10 hours. As in the July 9 experiment, if no HC reactions had occurred, both sides of this experiment would have had the same *final* NMHC concentration and composition. *During* the experiment, however, the total NMHC concentration and composition would have been different. The outcome of this experiment was not what we expected; that is, we were surprised that the two sides with such different concentration and composition NMHC, were essentially matched in the NO_x and O_3 chemistry.

Another experiment was conducted on August 22, 1983 which added another dimension to the experiment of July 9 discussed above. The conditions were the

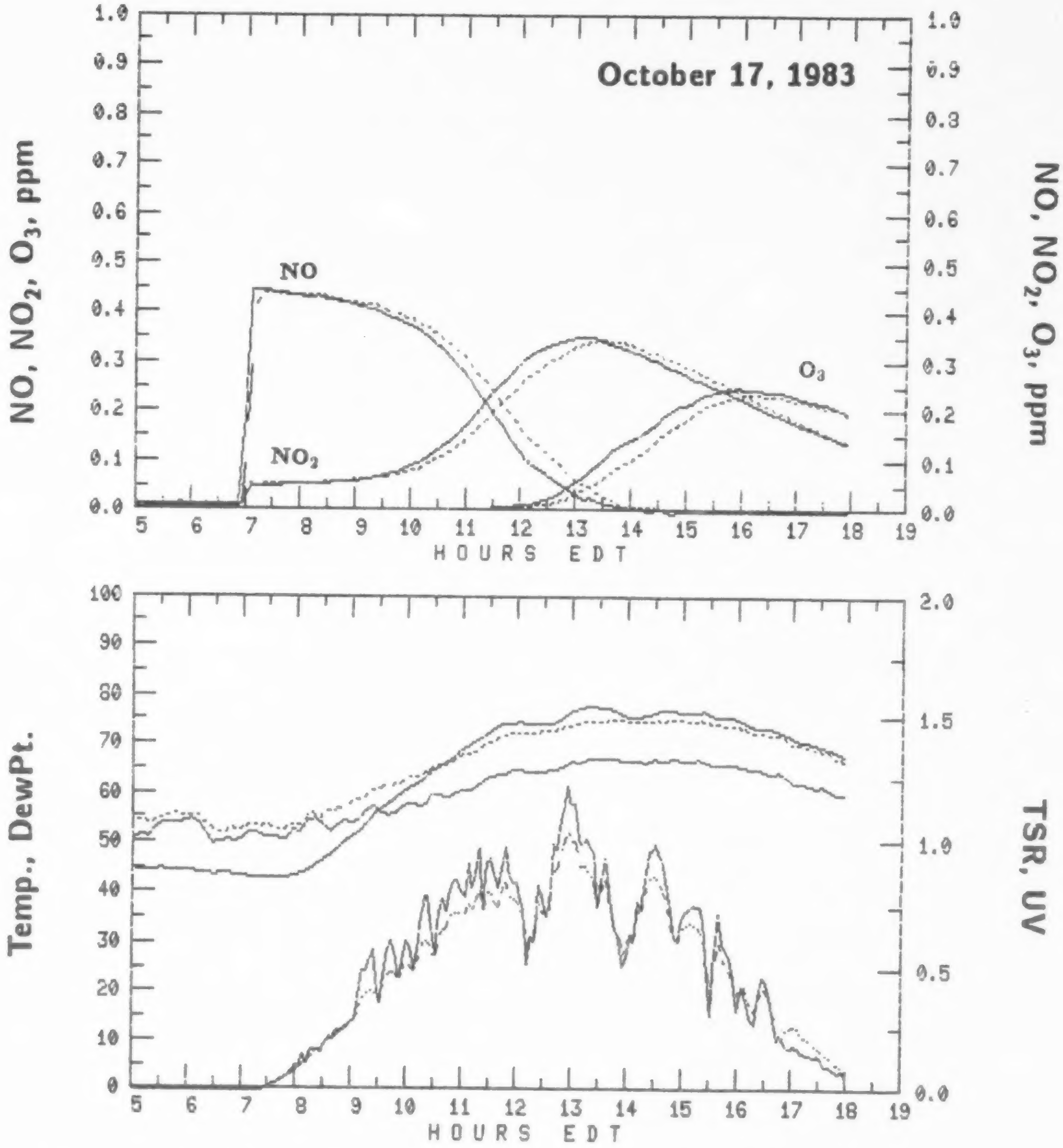

Figure 19. TOP: Static Injections of 1.0 ppmC isopentane, 1.0 ppmC 2,2,4-trimethylpentane, 0.82 ppmC toluene, 0.4 ppmC m-xylene and 0.46 ppm NO_x with CSTR Injection of 1.1 ppmC propylene (Dashed Line) and Static Injections of 1.1 ppmC propylene, 0.82 ppmC toluene, 0.4 ppmC m-xylene and 0.46 ppm NO_x with CSTR Injection of 1.0 ppmC isopentane, 1.0 ppmC 2,2,4-trimethylpentane (Solid Line). BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation.

same as the July 9 experiment except that on one side NO_x was injected continuously instead of initially.

EKMA type Model Tests

Chemical species used in EKMA-type mechanisms usually are of two types: specific species which have unique characteristics and generally represent themselves, and surrogate or lumped species that represent a whole class of compounds. Testing of such chemical mechanisms requires smog chamber experiments different than those used for testing mechanisms only comprised of explicit species. Experiments with a representative set of compounds are needed for testing the representation provided by surrogate species.

More complex mixtures are needed to test the chemistry of lumped or generalized compounds. Several mixtures, such as synthetic automobile exhaust or surrogate atmospheric mixtures, have been used to test mechanisms of this type. The composition of these mixtures are given in Tables 10 and 11. These HC mixtures were based on analysis of published atmospheric and automobile exhaust data using a computer program written by Sexton. The program ranks the major compounds by class and calculates average carbon numbers for each class. In addition, it lists the compounds that make up a given fraction of each class. In constructing synthetic mixtures, compounds can be selected that not only represent the major HC classes but also approximate the distribution of compounds within a class. Table 30 is an example of selecting the major compounds from one of the atmospheric analyses.[23] In this case, each group listed contains the compounds that comprise 75% of the total carbon in each class, *i.e.* 8 compounds make up 75% of the paraffins.

The mixtures named in Tables 10 and 11 contain species explicitly represented in chemical mechanisms as well as compounds that are usually "lumped". These mixtures also vary in complexity. The compositions vary within hydrocarbon class (eg. toluene-to-aromatic ratio or non-toluene, mono-alkyl aromatics-to-aromatics ratios). These experiments provide a more reasonable test of both the explicit and lumped species. Experiments conducted with explicit species as the only portion of a HC class or as a reference condition in one side of a dual-experiment can provide a convenient transition point from explicit to lumped species testing. For example, an aromatic mixture is conveniently tested in a propylene/butane matrix (July 8, 1982). The propylene/butane mixture compares easily to a complex mix of olefins and paraffins (*e.g.* UNCMIX).

UNCMIX is an eleven component mixture of olefins and paraffins based on atmospheric measurements in Los Angeles.[23] It is used extensively throughout the

Table 30. Analysis of Gas Chromatographic Data Of Los Angeles (Kopczynski) 75% Of Each Major HC Class

ID NUM.	COMPOUND	CAR. FRACTION
17	ISOPENTANE	0.0917
12	N-BUTANE	0.0840
3	ETHANE	0.0561
19	N-PENTANE	0.0502
6	PROPANE	0.0411
38	2,4-DIMETHYLPENTANE	0.0262
33	N-HEXANE	0.0241
25	CYCLOPENTANE	0.0203
55	TOLUENE	0.0796
68	M-XYLENE	0.0632
67	P-XYLENE	0.0294
71	O-XYLENE	0.0256
78	1,2,4-TRIMETHYLBENZENE	0.0201
79	SEC-BUTYLBENZENE	0.0201
65	ETHYLBENZENE	0.0197
2	ETHYLENE	0.0444
5	PROPYLENE	0.0176
83	2-METHYL-2-BUTENE	0.0085
10	1-BUTENE	0.0069
11	ISOBUTYLENE	0.0069
21	TRANS-2-PENTENE	0.0065
4	ACETYLENE	0.0470

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HC ANALYSIS FOR KOPLAM.HC
 45 COMPOUNDS TOTAL  TOTAL "CONCENTRATION" =  3.403000E+03
 OLE FRAC 0.1131  OLE CARBON NUM.  2.8861  13 COMPOUNDS
 PAR FRAC 0.5040  PAR CARBON NUM.  4.1363  15 COMPOUNDS
 ARO FRAC 0.3341  ARO CARBON NUM.  8.2082  15 COMPOUNDS
```

UNC data set. SIMARO ("simple" aromatic) and COMARO ("complex" aromatic) are two often used aromatic mixtures. COMARO is the complementary aromatic portion of the olefin-paraffin mixture UNCMIX.

UNCMIX provides a good test of olefin and paraffin chemistry, containing a wide range of compound types within each class. Compounds often represented explicitly, such as ethylene and propylene are also included.

Table 31 lists experiments that are useful in testing models designed for EKMA use. Selected experiments from this list are described below.

The dual-experiment conducted on June 15, 1982 compared a UNCMIX-NO_x system with a matched mass system with COMARO substituted for the paraffin/olefin carbon.

The October 7, 1983 experiment, shown in Figure 20 compared the UNCMIX-COMARO-NO_x system with a 13-component synthetic auto exhaust which has been demonstrated to be similar in reactivity to real auto exhaust.[15] Models should be able to simulate the range of reactivity caused by the compositional difference between these two sides.

The experiment conducted on September 20, 1981 was a matched NMHC-NO_x experiment using the UNCMIX with aromatics substituted. The two sides had an equal aromatic substitution: SIMARO on one side and COMARO on the other side.

Two substitution experiments using SIMARO that was substituted with two different olefin-paraffin mixtures which differed in complexity and types of compounds within each class were also performed. UNCMIX and SIMMIX1 are compared in the experiment conducted August 26, 1981. A similar experiment was conducted July 19, 1982 with SIMMIX2 which is like SIMMIX1 but minus the propylene.

The September 2, 1981 experiment demonstrated the effects of variation of HC class fractions. The aromatic fractions are varied while maintaining the same relative ratio of olefin to paraffin. Two UNCMIX-NO_x systems with different substitution levels of SIMARO were compared in this experiment.

The experiments of September 10 and 12, 1981 were comparisons of two UNCMIX-SIMARO-NO_x systems with n-butane added to one side to vary both the overall relative HC class fractions and the internal alkane composition. The added n-butane

Table 31 EKMA Model Test Runs

RUN DATE		NOX	HC		Proj.	Q	I	P
26-Aug-81	O N I	0.711	1.46	UNCMIX	REAC	8	5	S
			0.56	SIMARO				
		0.235	1.37	SIMMIX1				
			0.58	SIMARO				
2-Sep-81	O N I	0.246	2.04	UNCMIX	REAC	7	3	S
			0.43	SIMARO				
		0.247	1.62	UNCMIX				
			0.75	SIMARO				
20-Sep-81	O N I	0.238	1.62	UNCMIX	REAC	9	3	S
			0.65	COMARO				
		0.229	1.57	UNCMIX				
			0.51	SIMARO				
13-Nov-81	O N I	0.500	2.73	UNCMIX	REAC	9	0	P
			1.18	SIMARO				
			0.04	ACETALDEHYDE				
		0.500	4.00	DODGEMIX II				
8-Jul-82	O N I	0.291	1.19	BUTANE/PROPYLENE	REAC	9	7	S
			0.89	SIMARO				
		0.283	1.08	BUTANE/PROPYLENE				
			1.03	COMARO				
19-Jul-82	O N I	0.294	2.10	UNCMIX	REAC	6	7	S
			0.60	COMARO				
		0.291	2.07	SIMMIX2				
			0.60	COMARO				
22-Jul-82	O N I	0.300	3.50	SIMARO	REAC	2	5	L
		0.300	2.90	COMARO				

23-Sep-82	O N I	0.400	2.10	UNCMIX	REAC	9 4 L
			0.90	SIMARO		
		0.400	2.10	UNCMIX		
			0.90	COMARO		
7-Oct-83	O N I	0.334	1.89	UNCMIX	AURE	8 8 S
			0.75	COMARO		
		0.345	2.69	SYNTHETIC AUTO EXHAUST		
15-Jun-82	O N I	0.320	3.40	UNCMIX	REAC	8 7 S
		0.312	2.54	UNCMIX		
			0.86	COMARO		
7-Dec-82	O N I	0.187	2.47	UNCMIX	REAC	9 6 S
			0.90	COMARO		
		0.186	3.49	UNCMIX		
27-Aug-81	O N I	0.234	2.11	SIMMIX1	REAC	7 4 S
		0.233	1.43	SIMMIX1		
			0.58	SIMARO		
3-Sep-81	O N I	0.235	1.78	UNCMIX	REAC	7 4 S
			0.53	SIMARO		
		0.231	1.40	UNCMIX		
			0.46	SIMARO		
			0.57	PROPYLENE		
10-Sep-81	O N I	0.235	2.79	UNCMIX	REAC	7 3 S
			0.70	SIMARO		
		0.246	1.02	UNCMIX		
			0.50	SIMARO		
			2.21	N-BUTANE		
12-Sep-81	O N I	0.251	1.68	UNCMIX	REAC	7 4 S
			0.55	SIMARO		
		0.285	1.14	UNCMIX		
			0.39	SIMARO		
			0.62	N-BUTANE		

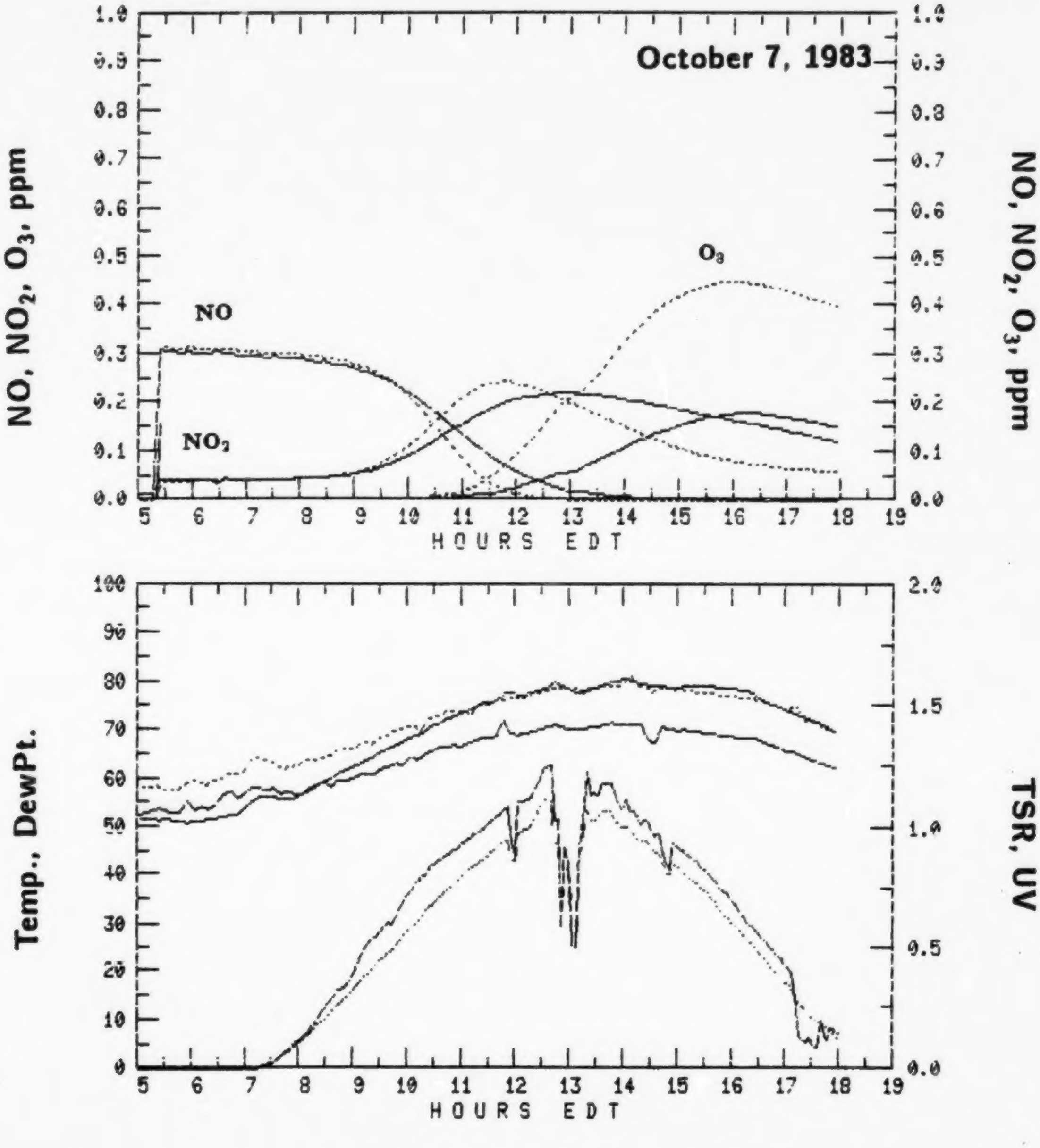

Figure 20 TOP: Synthetic Auto Exhaust, NMHC= 2.69 ppmC, (dashed lines); Synthetic Urban Mixture, NMHC= 2.65 ppmC, (solid lines).
BOTTOM: Chamber air temperature and dew point; ambient total solar and ultraviolet radiation;

chemistry increased the straight to branched alkane ratio, and shortened the average carbon number for the alkane class. The experiment of September 3, 1981 was similar to the butane experiments; however, propylene was substituted in one side.

General "lumped" chemistry mechanisms can be tested against several dynamic runs that were conducted in this program. For example, the dual-experiment conducted on October 6, 1983 simulated two different atmospheric dilution rates of otherwise matched static injection systems of UNCMIX and four aromatics. A 50% reduction EKMA test with continuous injections simulating continuous emissions used a modified UNCMIX (extra branched alkanes) with another aromatic mixture (September 12, 1983).

7

Obtaining Data For Runs

Changing Database

The data set described in this report is neither complete nor static. The data were produced in a series of co-ordinated projects. New projects are currently adding experiments to the data set; these newer experiments are not described here. The organizing methods described herein, however, will be applied to these experiments and they will be added to the Experimental Conditions Database and the run data will be made available to modelers.

In spite of these new experiments, needed experimental conditions are still missing and model testing often reveals the need for new conditions not in the data set. Thus, the data set is planned to grow for some time.

Meanwhile, the existing runs are under constant review and analysis. Not only are we using the data ourselves, but two EPA-sponsored model testing groups are currently using the data. Thus, even the information presented in this report is likely to change as runs are reviewed and compared to newer runs.

In a data set as large as this one, errors will be present in spite of extensive Quality Assurance procedures (see reference 15). As we find errors in the data set or the Experimental Conditions Database, we correct them. These errors generally concern the exact initial concentrations of reactants. Revisions of calibration factors can change the concentrations actually reported in the data set. Sometimes these changes are not reflected in the Experimental Conditions Database. Users are cautioned to consult the actual data in the magnetic tape data set for the exact initial concentrations. The values in the Experimental Conditions Database are useful only for selecting runs.

Another change to the database is the processing status of runs. Older and sometimes excellent runs are being further processed and placed on the magnetic data tape as time permits. These appear in the Experimental Conditions Database as "P" runs (those currently being processed) or "L" runs (those that are processable but have a lower priority).

As the series of outdoor smog chamber experimental projects evolved, so did the sophistication of data production, data processing, and data packaging. Thus not all the data are in exactly the same format. Although the formats are quite similar, this problem is still a nuisance. As time permits, the "Best" of the older runs are being converted to the newer format.

The Magnetic Data Tape

Fully processed runs, those with a processing status of "S" in the Experimental Conditions Database, are placed on a nine-track, American National Standards Institute (ANSI) formatted magnetic tape. This type of format can be easily read on IBM machines using OS/370 version operating systems and on DEC VAX machines using VMS operating systems, the two most common machines. Since it is a national standard format, it is also most likely readable on many other manufactor's machines. (Our tapes also have been read on PRIME and on UNIVAC machines.)

All data for a given day appear in a single file, called a *SegFile* (segmented file format). This format allows extensive documentation to be included with the actual run data and collects all the different types of data into a single entity. The exact format of the data files is given in "Format of UNC Outdoor Smog Chamber Data Files and Magnetic Tape," a document that is supplied with the data tape.

Copies of the data tape, other supporting information, and the Experimental Conditions Database can be obtained by telephoning or writing

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There is a media and distribution fee for producing a data tape and documentation.

Assistance, Suggestions

The authors welcome suggestions from users on formats, documentation, and other issues related to the ease of use of the data.

The authors can also provide assistance by answering questions about experimental runs and can offer suggestions on special test situations and run selections.

References

1 Freas, W.P., Martinez, E.L., Meyer, E.L., Possiel, N.C., Sennet, D.H., Summerhays, J.E, "Procedures for quantifying Relationships Between Photochemical Oxidants and Precursors: Supporting Documentation" EPA-450/2-77-021b, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1978.

2 Gipson, G.L. "Guideline For Using The Carbon-Bond Mechanism In City-Specific EKMA" EPA-450/4-84-005, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1984.

3 Jeffries H.E., Sexton K.G., Salmi C.N. "The Effects of Chemistry and Meteorology on Ozone Control Calculations Using Simple Trajectory Models and the EKMA Procedure" EPA-450/4-81-034, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1981.

4 Killus J.P., Whitten G.Z., "Effects Of Photochemical Kinetics Mechanisms on Oxidant Model Predictions", EPA-600/3-83-111, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1983.

5 Carter W.P.L., Winer A.M., Pitts, Jr. J.N., "Effects of Mechanism and Hydrocarbon Compositions on Oxidant-Precursor Relationships Predicted by the EKMA Isopleth Technique", *Atmos. Envr.*, **16**, 113—120, 1982.

6 Leone J.A., Seinfeld, J.H., "Evaluation of Chemical Reaction Mechanisms for Photochemical Smog: Part II. Quantitative Evaluation of The Mechanisms", EPA-600/3-84-063, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1984.

7 Jeffries H.E., "A Photochemical Reaction Mechanism Analysis Method Applied to Two Mechanisms", submitted *Envr. Sci. and Techno.*, Nov. 1984.

8 Whitten G.Z. "The Chemistry of Smog Formation: A Review of Current Knowledge,", *Environment International* **9**, 447–463, 1983.

9 Atkinson R., Lloyd A.C. "Kinetic and Mechanistic Data for Modeling of Photochemical Smog", *J. Phys. Chem. Ref. Data*, **13**, 315—444, 1984.

10 Atkinson R., Lloyd A.C, Winges, L.,"An Updated Chemical Mechanism for Hydrocarbon/ NO_x Photooxidations Suitable for Inclusion in Atmospheric Simulation Models", *Atmos. Envr.*, **16**, 1341—1355, 1982.

11 Gery, M.W., Fox. D.L., Jeffries, H.E., "A Continuous Stirred Tank Reactor Investigation of the Gas Phase Reaction of Hydroxyl Radicals and Toluene" *Int. J. Chem. Kinet.*, in press, January 1985.

12 Jeffries H.E., Kamens R.M., Sexton K.G., and Gerhardt A.A., "Outdoor Smog Chamber Experiments To Test Photochemical Models", EPA-600/3-83-016a, U.S. Environmental Protection Agency, Research Triangle Park, N.C., 1982

13 Jeffries H.E., Kamens R.M., Sexton K.G., and Gerhardt A.A., "Outdoor Smog Chamber Experiments To Test Photochemical Models", NTIS Order No. *PB 82-198 508*

14 Jeffries, H.E. "Modeling Observed Hydrocarbon Mixture Reactivity Effects", Technical Narrative, EPA Grant Request 807762, 1981

15 Jeffries H.E., Sexton K.G., Morris, T.P., Jackson M., Goodman R.G., Kamens R.M., Holleman M.S, "Outdoor Smog Chamber Experiments Using Automobile Exhaust", Final Report for Cooperative Agreement 809391, Environmental Protection Agency, Research Triangle Park,

N.C., 1985

16 Jeffries H.E., Sexton K.G., "Smog Chamber Background Reactivity, Part1: The Influence of NO_x from Chamber Walls on Kinetic Computer Models for Air Pollution," submitted *Atmospheric Environment*, March 1983

17 Jeffries H.E., Sexton K.G., "Smog Chamber Background Reactivity, Part2: The Influence of Radicals from Chamber Walls on Kinetic Computer Models for Air Pollution," submitted *Atmospheric Environment*, March 1983

18 Whitten G.Z., Killus J.P., Johnson R.G., "Modeling of Simulated Photochemical Smog with Kinetic Mechanisms," EPA-600/3-83-043, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1983

19 Killus J.P., Whitten G.Z., "Technical Discussion Relating To the Use of The Carbon Bond Mechanism in OZZIP/EKMA," EPA-450/4-84-009, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1984

20 Gery M.W. "CSTR Investigations of Aromatic OH Reactions", Ph.D. Dissertation, University of North Carolina, Chapel Hill, N.C., 1985.

21 Fox D.L., Kamens R.M., Jeffries H.E. "Photochemical Smog Systems: Heterogeneous Decay of Ozone" *Science* **191** No. 4231, p.1058, 1976.

22 Sexton, K.G., "Experimental Simulation of Urban-Like Smog System for Studying the Chemistry of Ozone Formation," Ph.D. Dissertation, University of North Carolina, Chapel Hill, 1984.

23 Kopczynski S.L., Lonneman W.A., Sutterfield F.D., Darley P.E., "Photochemistry of Atmospheric Samples in Los Angeles" *Envron. Sci. and Tech.* **6**, 342–350, 1972.

A

Exp. Cond. Database

This appendix lists the Experimental Conditions Database. This database is available on several forms of magnetic media:

- 9-track ANSI standard labeled magnetic tape;
- DEC RT-11-formatted, single density, 8" floppy disk;
- DEC VAX/VMS-formatted, single density, 8" floppy disk;
- IBM PC-DOS (MS-DOS) formatted, single-sided, 5.25" floppy disk readable on IBM PC, XT, AT personal computers.

Using this database modelers can quickly locate experiments that meet their particular testing needs. The experimental data for the selected runs can then be loaded from the magnetic tape.

Table 32 describes the data fields in each record. To keep these records short, codes have been used for many of the fields, especially for the HC species and mixture names. The translations of the codes for these fields are given in Table 33. A more detailed description of these codes was given in Table 3 in Chapter 2. A list of HC codes and associated names is given in Table 34.

Although it is expected that users will place this database on a computer and use a database query language capable of easily translating the codes into english for reports, the database is not that difficult to search by hand, therefore, the database is listed here as a printout in Table 35 in chronological order.

Table 32. The format of the Experimental Conditions Database.

Column	Field Name	Units or Code
1–6	Run Date	YYMMDD
8	Class	see Table 33
9	Dilution	see Table 33
10	Injection	see Table 33
11–12	HC-type	see Table 33
14–48	RED Side Initial Concentrations	
14–18	Initial NO_x concentration	ppm
20–28	First HC species or mixture	
20–24	Initial HC concentration	ppmC
26–28	HC species/mixture code	see Table 34
30–38	Second HC species or mixture	
30–34	Initial HC concentration	ppmC
36–38	HC species/mixture code	see Table 34
40–48	Third HC species or mixture	
40–44	Initial HC concentration	ppmC
46–48	HC species/mixture code	see Table 34
50–84	BLUE Side Initial Concentrations	
50–54	Initial NO_x concentration	ppm
56–64	First HC species or mixture	
56–60	Initial HC concentration	ppmC
62–64	HC species/mixture code	see Table 34
66–74	Second HC species or mixture	
66–70	Initial HC concentration	ppmC
72–74	HC species/mixture code	see Table 34

Column	Field Name	Units or Code
76–84	Third HC species or mixture	
76–80	Initial HC concentration	ppmC
82–84	HC species/mixture code	see Table 34
86–87	Project Code	see Table 33
88	Number of HC inst. used	
89	Processing Status	see Table 33
90	Overall Quality	0–9 (highest)
92–94	Series1	see Table 33
95–97	Rank in series1	1 (first) to 999 (lowest)
99–101	Series2	see Table 33
102–104	Rank in series2	1 (first) to 999 (lowest)
106–108	Series2	see Table 33
109–111	Rank in series2	1 (first) to 999 (lowest)

Table 33. Codes used in the Experimental Conditions Database.

Code	Meaning
	Class Codes
C	characterization experiment
D	characterization experiment, second day
O	one day organic/NO_x experiment
T	two day organic/NO_x experiment
S	second day of two day organic/NO_x experiment
	Dilution Codes
N	normal dilution; 1% per hour
D	large dilution: *e.g.* five-fold
	Injection Codes
I	initially injected only
H	HC continuously injected
N	NO_x continuously injected
B	both HC and NO_x continuously injected
C	some other combination

Table 33. Codes used in the Experimental Conditions Database, cont.

Code	Meaning
	HC Type Codes
1A	single aldehyde each side
1O	single olefin each side
1P	single paraffin each side
1R	single aromatic each side
1U	olefin one side, aldehyde other side
1V	olefin one side, paraffin other side
1W	olefin one side, aromatic other side
1X	some other combination
MB	simple mixture of 2 or 3 species
MC	complex mixture or mixture of mixtures
MV	mixture with time varying composition
B	background air
S	only one side used
	Project Identification Codes
ET	Experiments to Test Photochemical Models
RE	Reactivity
AU	Automobile exhaust
	Processing Status Codes
S	fully processed; segfile
P	partially processed
L	partially processed;low priority
N	not to be processed
U	unprocessed run
	(blank state) status unknown

Table 33. Codes used in the Experimental Conditions Database, cont.

Code	Meaning
	Series Codes
1	Characterization; Background
2	Characterization; NO oxid. NO only
3	Characterization; NO oxid. CO added
4	Characterization; O3 decay
5	Characterization; NO2/O3, dark
6	Characterization; Ald. added
7	Matched propylene
8	Matched mixture
9	Matched other
10	Replicate propylene
11	Replicate other
12	Aldehyde developement
13	Olefin developement
14	Paraffin developement
15	Aromatic developement
16	HC type transition
17	Terpene developement
18	Reactivity Comparison
19	Single to Simple
20	Simple Comp. Change
21	Complex Comp. Change
22	Simple to Complex
23	Substitution, UNCMIX
24	Substitution, P/B
25	Substitution, SIMMIX
26	Substitution, Other
27	Addition, one species
28	Addition, CO
29	Addition, Ald
30	Addition, Other

Table 33. Codes used in the Experimental Conditions Database, cont.

Code	Meaning
	Series Codes, cont.
31	AutoExhaust
32	EKMA test
33	Delta HC
34	Delta NOx
35	Static to dynamic
36	Temperature effects
37	Water effects
38	Solar effects
39	Ketone developement
40	All NO2

Table 34

Species Identification Numbers

ID NUMBER	SPECIES NAME	CARBON NUMBER	CLASS
1	METHANE	1	M
2	ETHYLENE	2	O
3	ETHANE	2	P
4	ACETYLENE	2	Y
5	PROPYLENE	3	O
6	PROPANE	3	P
7	PROPADIENE	3	D
8	METHYL ACETYLENE	3	Y
9	ISOBUTANE	4	P
10	1-BUTENE	4	O
11	ISOBUTYLENE	4	O
12	N-BUTANE	4	P
13	1,3-BUTADIENE	4	D
14	TRANS-2-BUTENE	4	O
15	CIS-2-BUTENE	4	O
16	3-METHYL-1-BUTENE	5	O
17	ISOPENTANE	5	P
18	1-PENTENE	5	O
19	N-PENTANE	5	P
20	2-METHYL-1-BUTENE	5	O
21	TRANS-2-PENTENE	5	O
22	CIS-2-PENTENE	5	O
23	2,2-DIMETHYLBUTANE	6	P
24	CYCLOPENTENE	5	C
25	CYCLOPENTANE	5	E
26	3-METHYL-1-PENTENE	6	O
27	2,3-DIMETHYLBUTANE	6	P
28	2-METHYLPENTANE	6	P
29	2,3-DIMETHYL-1-BUTENE	6	O
30	3-METHYLPENTANE	6	P
31	1-HEXENE	6	O
32	2-ETHYL-1-BUTENE	6	O
33	N-HEXANE	6	P
34	CIS-3-HEXENE	6	O
35	2-METHYL-2-PENTENE	6	O
36	METHYLCYCLOPENTANE	6	E
37	3-METHYLTRANS-2-PENTENE	6	O
38	2,4-DIMETHYLPENTANE	7	P
39	METHYLCYCLOPENTENE	6	C
40	BENZENE	6	A
41	CYCLOHEXENE	6	C
42	2,3-DIMETHYLPENTANE	7	P
43	2-METHYLHEXANE	7	P
44	3-METHYLHEXANE	7	P
45	CYCLOHEXANE	6	E
46	ISOOCTANE	8	P
47	N-HEPTANE	7	P
48	2,4,4-TRIMETHYL-1-PENTENE	8	O
49	METHYLCYCLOHEXANE	7	E
50	1-CIS-4-DIMETHYLCYCLOHEXANE	8	E
51	2,4-DIMETHYLHEXANE	8	P
52	2,5-DIMETHYLHEXANE	8	P
53	2,3,4-TRIMETHYLPENTANE	8	P
54	2,3,3-TRIMETHYLPENTANE	8	P
55	TOLUENE	7	A
56	2,3-DIMETHYLHEXANE	8	P
57	2-METHYLHEPTANE	8	P
58	3-METHYLHEPTANE	8	P
59	2,2,5-TRIMETHYLHEXANE	9	P
60	N-OCTANE	8	P
61	2,3,5-TRIMETHYLHEXANE	9	P

Table 34 cont.

Species Identification Numbers

ID NUMBER	SPECIES NAME	CARBON NUMBER	CLASS
62	2,4-DIMETHYLHEPTANE	9	P
63	2,5-DIMETHYLHEPTANE	9	P
64	3,5-DIMETHYLHEPTANE	9	P
65	ETHYLBENZENE	8	A
66	2,3-DIMETHYLHEPTANE	9	P
67	P-XYLENE	8	A
68	M-XYLENE	8	A
69	4-METHYLOCTANE	9	P
70	3-METHYLOCTANE	9	P
71	O-XYLENE	9	A
72	NONANE	9	P
73	N-PROPYLBENZENE	9	A
74	1-METHYL 3-ETHYL-BENZENE	9	A
75	1-METHYL 2-ETHYL-BENZENE	9	A
76	MESITYLENE	9	A
77	2,6-DIMETHYLOCTANE	10	P
78	1,2,4-TRIMETHYLBENZENE	9	A
79	SEC-BUTYLBENZENE	10	A
80	N-DECANE	10	P
81	UNKNOWNS	10	U
82	2,2,4-TRIMETHYLPENTANE	8	P
83	2-METHYL-2-BUTENE	5	O
84	M-ETHYLTOLUENE	10	A
85	P-ETHYLTOLUENE	10	A
86	O-ETHYLTOLUENE	10	A
87	TERT-BUTYLBENZENE	10	A
88	ISOPROPYLBENZENE	9	A
89	STYRENE	8	A
90	CIS-1,3-DIMETHYLCYCLOPENTANE	7	E
91	TRANS-1,3-DIMETHYLCYCLOPENTANE	7	E
92	UNDECANE	11	P
93	ISOPRENE	5	D
94	CIS-4-METHYL-2-PENTENE	6	O
95	TRANS-2-HEXENE	6	O
96	CIS-2-HEXENE	6	O
97	TRANS-4-METHYL-2-PENTENE	6	O
98	ISONONANE	9	P
99	1,2,3-TRIMETHYLBENZENE	9	A
100	BUTYLBENZENE	10	A
101	DIMETHYLETHYLBENZENE	10	A
102	3,3-DIMETHYL-1-BUTENE	6	O
103	2-ETHYL-1-BUTENE	6	O
104	TRANS-3-HEXENE	6	O
105	2,2-DIMETHYLPENTANE	7	P
106	2,3-DIMETHYL-2-BUTENE	6	O
107	2,3,3-TRIMETHYL-1-BUTENE	7	O
108	3,3-DIMETHYLPENTANE	7	P
109	2-METHYL-CIS-3-HEXENE	7	O
110	2,3-DIMETHYL-1-PENTENE	7	O
111	2,4-DIMETHYL-2-PENTENE	7	O
112	A-PINENE	10	T
113	CIS-4-METHYL-2-PENTENE	6	O
114	2,2,3-TRIMETHYLPENTANE	8	P
115	3-ETHYLHEXANE	8	P
116	ETHYLCYCLOHEXANE	8	E
117	A-METHYLSTYRENE	9	A
118	1,3-DIETHYLBENZENE	10	A
119	1,4-DIETHYLBENZENE	10	A
120	1,2-DIETHYLBENZENE	10	A
121	3-METHYL-2-BUTENE	5	O
122	4-METHYL-1-PENTENE	6	O

Table 34 cont.

Species Identification Numbers

ID NUMBER	SPECIES NAME	CARBON NUMBER	CLASS
123	2-METHYL-1-PENTENE	6	O
124	2,2,3-TRIMETHYLBUTANE	7	P
125	ETHYLCYCLOPENTANE	7	E
126	B-PINENE	10	T
127	LIMONENE	10	T
128	D-3-CARENE	10	T
129	B-PHELLANDRENE	10	T
130	MYRCENE	10	T
131	3-METHYLCIS-2-PENTENE	6	O
132	DODECANE	12	P
133	TRIDECANE	13	P
134	TETRADECANE	14	P
138	PAN	1	N
139	FORMALDEHYDE	1	L
146	METHACROLEIN	4	L
147	METHYLVINYLKETONE	4	K
148	ACETALDEHYDE	2	L
149	2-HEXENE	6	O
150	3,3 DIMETHYL-1-BUTENE	6	O
151	2,4,4 TRIMETHYLPENTENE	8	O
152	PENTADECANE	15	P
153	NAPHTHALENE	10	A
154	1,3,5-TRIMETHYLBENZENE	9	A
155	1,4-DIOXANE	4	X
156	2,2,5-TRIMETHYLPENTANE	8	P
157	4-METHYLHEPTANE	8	P
158	ACETONE	3	K
159	BUTYL CELLOSOLVE	6	X
160	BUTYLALDEHYDE	4	L
161	ACROLEIN	3	L
162	BENZALDEHYDE	6	L
163	ETHYLACETYLENE	4	Y
164	ETHYLENE GLYCOL	2	X
165	GLYCOL	2	X
166	HEXADECANE	16	P
167	METHYL CELLOSOLVE	3	X
168	METHYL ETHYL KETONE	4	K
169	METHYL ISOBUTYL KETONE	6	K
170	METHYL N-BUTYL KETONE	6	K
171	PHENOLS	6	X
172	PROPIONALDEHYDE	3	L
174	TETRAMETHYLBENZENE	10	A
175	2-METHYL-1,3-BUTADIENE	5	D
176	2-METHYLOCTANE	9	P
177	TRANS-2-NONENE	9	O
178	2,3-DIMETHYLOCTANE	10	P
179	METHYL CYCLOOCTANE	9	E
180	CIS-PROPYLBENZENE	9	A
181	INDANE	9	A
182	4-PHENYL-1-BUTENE	10	A
183	1-METHYL-3N-PROPYLBENZENE	10	A
184	2-METHYLDECANE	11	P
185	CYCLOPENTYLCYCLOPENTANE	10	E
186	1-UNDECENE	11	O
187	TRANS-1-PHENYLBUTENE-1	10	A
188	HEXYNE	6	Y
189	PENTYNE	5	Y
196	BIACETYL		
197	METHYLGLYOXAL		
198	METHYLBENZYLQUINONE		
200	N-PROPYLNITRATE		

Table 34 cont.

Species Identification Numbers

ID NUMBER	SPECIES NAME	CARBON NUMBER	CLASS
201	N-BUTYLNITRATE		
202	3-PENTANONE	5	K
203	GLYCOALDEHYDE		
204	ACETONITRILE	2	N
205	METHANOL	1	H
208	1-METHYLNAPHTHALENE		
211	2-METHYLNAPHTHALENE		
215	ETHYLNITRATE		
218	GLYOXAL		
219	TOLUALDEHYDE		
220	BUTYLNITRATE		
221	PROPYLNITRATE		
414	PPN		
416	TETRACHLOROETHYLENE		
417	TRICHLOROTRIFLUOROETHANE		
435	NO	1	N
436	NO2	1	N
437	O3	3	Z
438	NOX		
440	TSR	1	S
441	UV	1	S
442	CO	1	R
443	TEMP	1	F
444	DEW POINT	1	F
445	CC14	1	?
446	H2O2	0	
447	N2O	0	N
600	CH4ASTHC		
601	NMHCASTHC		
602	AUTO EXHAUST		
603	SYNTHETIC AUTO EXHAUST		
604	'72 DODGE AUTO EXHAUST DIRECT		
605	'72 DODGE AUTO EXHAUST CRYO		
606	'79 VOLARE AUTO EXHAUST DIRECT		
607	'79 VOLARE AUTO EXHAUST CRYO		
608	SYNTHETIC AUTO EXHAUST 0		
609	SYNTHETIC AUTO EXHAUST 1A		
610	SYNTHETIC AUTO EXHAUST 1B		
611	NO2 AS PAN		
612	BHC		
620	NMHC-RED		
621	NMHC-BLUE		
673	TERPENES	10	T
681	TOL/XYL/MIX1		
682	TOL/XYL/MIX2		
683	TOL/XYL/MIX3		
684	TOL/TMB/XYLS		
685	ISO-/2,2,4-TM-PENTANES		
690	THC	5	H
691	UNCMIX		
692	SIMMIX1		
693	COMARO		
694	SIMARO		
695	BUTANE/PROPYLENE		
696	SIMMIX2		
698	AROMATIC MIX		
699	DODGEMIX II		
998	TWO DAY CON'T		
999	BACKGROUND		

Table 35.

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                    UNC Outdoor Smog Chamber Experimental Conditions Database

Column Numbers:

                                                                                                      11111  111111
          111  11111 22222 222 33333 333 44444 444 55555 55556 666 66667 777 77778 888 88889 999999 900000 000011
123456 89012 45678 01234 678 01234 678 01234 678 01234 67890 234 67890 234 67890 234 67890 234567 901234 678901

770518 ONI1A 0.359 01.07 140 00.00 000 00.00 000 0.357 01.10 139 00.00 000 00.00 000 ET0S8 018075 000000 000000
770603 ONIMB 0.351 01.60 005 00.50 139 00.00 000 0.345 01.69 005 00.00 000 00.00 000 ET0S7 029010 012000 012000
770718 ONI1A 0.539 01.21 139 00.00 000 00.00 000 0.535 01.00 140 00.00 000 00.00 000 ET0S9 018001 012001 012001
770720 ONI1O 0.270 00.65 005 00.00 000 00.00 000 0.200 01.21 005 00.00 000 00.00 000 ET0S8 033010 000000 000000
770727 ONI1A 0.552 01.00 139 00.00 000 00.00 000 0.550 00.55 140 00.00 000 00.00 000 ET0S5 018051 000000 000000
770728 ONI1A 0.526 01.16 139 00.00 000 00.00 000 0.529 02.20 139 00.00 000 00.00 000 ET0S5 033999 000000 000000
770808 ONI1O 0.499 01.54 005 00.00 000 00.00 000 0.501 01.50 005 00.00 000 00.00 000 ET0S5 007005 000000 000000
770914 ONI1A 0.397 01.05 139 00.00 000 00.00 000 0.009 01.20 139 00.00 000 00.00 000 ET0S4 034010 000000 000000
770919 ONI1A 0.382 01.00 139 00.00 000 00.00 000 0.386 00.60 139 00.00 000 00.00 000 ET0S3 033999 000000 000000
771012 ONI1O 0.505 03.56 005 00.00 000 00.00 000 0.501 01.72 005 00.00 000 00.00 000 ET0S4 033110 000000 000000
771018 ONI1O 0.494 03.04 002 00.00 000 00.00 000 0.484 01.80 002 00.00 000 00.00 000 ET0S6 033000 000000 000000
771022 ONI1V 0.518 03.69 005 00.00 000 00.00 000 0.525 00.10 012 00.00 000 00.00 000 ET0S6 018001 000000 000000
771024 ONI1V 0.517 03.69 005 00.00 000 00.00 000 0.490 00.00 012 00.00 000 00.00 000 ET0S5 018026 000000 000000
771109 ONI1O 0.529 03.77 005 00.00 000 00.00 000 0.537 01.92 005 00.00 000 00.00 000 ET0S7 033025 000000 000000
771112 ONI1U 0.503 02.00 002 00.00 000 00.00 000 0.471 01.72 140 00.00 000 00.00 000 ET0S6 018032 000000 000000
771119 ONI1U 0.451 03.78 002 00.00 000 00.00 000 0.832 03.82 140 00.00 000 00.00 000 ET0S7 018032 000000 000000
771120 ONI1U 0.446 04.37 002 00.00 000 00.00 000 0.881 03.92 140 00.00 000 00.00 000 ET0S8 018032 000000 000000
771226 ONI1U 0.399 02.96 005 00.00 000 00.00 000 0.407 03.82 140 00.00 000 00.00 000 ET0S9 018033 000000 000000
780110 ONI1O 0.462 03.25 005 00.00 000 00.00 000 0.482 04.35 002 00.00 000 00.00 000 ET0S8 018035 000000 000000
780120 ONIS  0.500 03.25 005 00.00 000 00.00 000 0.000 00.00 000 00.00 000 00.00 000 ET0S6 000010 036000 036000
780129 ONIS  0.477 03.20 005 00.00 000 00.00 000 0.000 00.00 000 00.00 000 00.00 000 ET0S6 000010 036000 036000
780227 ONI1U 0.496 03.95 005 00.00 000 00.00 000 0.354 01.90 140 00.00 000 00.00 000 ET0S7 018040 000000 000000
780306 ONI1U 0.511 03.77 005 00.00 000 00.00 000 0.374 01.80 140 00.00 000 00.00 000 ET0S5 018055 000000 000000
780331 ONI1U 0.483 03.82 005 00.00 000 00.00 000 0.393 02.00 140 00.00 000 00.00 000 ET0S6 018051 000000 000000
780616 ONI1O 0.634 03.95 002 00.00 000 00.00 000 0.640 02.00 005 00.00 000 00.00 000 ET0S7 010015 000000 000000
780618 ONIMC 0.354 02.27 012 00.75 005 00.00 000 0.354 03.20 691 00.00 000 00.00 000 ET0S7 018010 000000 000000
780621 ONIMC 0.357 01.05 691 00.00 000 00.00 000 0.353 01.50 012 00.54 005 00.00 000 ET0S6 018010 000000 000000
780701 ONI1O 0.887 01.45 002 00.00 000 00.00 000 0.935 01.51 005 00.00 000 00.00 000 ET0S7 018010 000000 000000
780721 ONI1P 0.243 07.30 012 00.00 000 00.00 000 0.242 15.70 012 00.00 000 00.00 000 ET0S8 033010 000000 000000
780722 ONI1P 0.540 08.34 012 00.00 000 00.00 000 0.557 17.50 012 00.00 000 00.00 000 ET0S8 033002 000000 000000
780724 ONI1O 0.959 02.97 005 00.00 000 00.00 000 0.952 01.47 005 00.00 000 00.00 000 ET0S7 033015 000000 000000
780727 ONI1P 0.266 13.50 012 00.00 000 00.00 000 0.509 13.20 012 00.00 000 00.00 000 ET0S5 034101 000000 000000
780730 ONI1O 0.474 01.32 002 00.00 000 00.00 000 0.403 01.25 005 00.00 000 00.00 000 ET0S6 018012 000000 000000
780805 ONI1O 0.240 00.83 005 00.00 000 00.00 000 0.560 01.55 005 00.00 000 00.00 000 ET0S4 033050 000000 000000
780806 ONI1O 0.561 01.69 005 00.00 000 00.00 000 0.569 02.59 002 00.00 000 00.00 000 ET0S4 018500 000000 000000
780808 ONI1A 0.516 00.91 140 00.00 000 00.00 000 0.527 04.00 140 00.00 000 00.00 000 ET0S4 033100 000000 000000
780811 CNIB  0.005 00.00 999 00.00 000 00.00 000 0.004 00.00 999 00.00 000 00.00 000 ET0S5 001020 000000 000000
780814 CNIB  0.522 00.00 999 00.00 000 00.00 000 0.523 00.00 999 49.20 442 00.00 000 ET0S6 003000 000000 000000
780816 ONI1O 0.543 01.45 005 00.00 000 00.00 000 0.563 01.58 002 00.00 000 00.00 000 ET0S7 010002 000000 000000
780816 ONI1W 0.687 01.56 006 00.00 000 00.00 000 0.691 03.93 055 00.00 000 00.00 000 ET0S7 018010 000000 000000
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Table 35 cont.

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780817 ONIIA 0.701 00.96 148 00.00 000 00.00 000 0.700 04.00 148 00.00 000 00.00 000 ET0S6 033010 000000 000000
780818 ONIIO 0.495 00.74 005 00.00 000 00.00 000 0.491 02.08 005 00.00 000 00.00 000 ET0S8 033002 000000 000000
780821 ONIIO 0.978 01.39 002 00.00 000 00.00 000 0.981 01.28 005 00.00 000 00.00 000 ET0S9 010013 000000 000000
780823 ONIIO 0.507 02.93 002 00.00 000 00.00 000 0.521 02.97 002 00.00 000 00.00 000 ET0S0 009010 000000 000000
780824 ONIIP 0.575 50.00 012 00.00 000 00.00 000 0.803 56.30 012 00.00 000 00.00 000 ET0S9 034010 000000 000000
780825 ONIIP 0.518 13.20 012 00.00 000 00.00 000 0.518 26.60 012 00.00 000 00.00 000 ET0S7 033036 000000 000000
780908 ONIIA 0.968 03.25 139 00.00 000 00.00 000 0.916 00.90 139 00.00 000 00.00 000 ET0S4 033500 000000 000000
780914 ONIIW 0.292 02.24 055 00.00 000 00.00 000 0.294 00.97 002 00.00 000 00.00 000 ET0S5 010015 000000 000000
780915 ONIIU 0.526 02.90 002 00.00 000 00.00 000 0.268 02.00 139 00.00 000 00.00 000 ET0S3 034100 000000 000000
780918 ONIIW 0.503 02.98 002 00.00 000 00.00 000 0.496 04.21 055 00.00 000 00.00 000 ET0S5 010065 000000 000000
780919 ONIIU 0.688 01.88 002 00.00 000 00.00 000 0.690 02.00 139 00.00 000 00.00 000 ET0S7 010051 000000 000000
780921 ONIIU 0.258 01.93 002 00.00 000 00.00 000 0.257 01.97 139 00.00 000 00.00 000 ET0S5 010051 000000 000000
781003 ONIMB 0.497 00.98 002 00.00 000 00.00 000 0.492 00.14 012 01.36 005 00.00 000 ET0S6 010035 000000 000000
781012 ONIMB 0.479 00.20 002 01.26 148 00.00 000 0.479 01.33 005 00.00 000 00.00 000 ET0S9 010035 000000 000000
781013 ONIIA 0.493 00.92 148 00.00 000 00.00 000 0.906 02.02 148 00.00 000 00.00 000 ET0S4 033050 000000 000000
781018 ONIIO 0.456 03.12 002 00.00 000 00.00 000 0.456 01.52 005 00.00 000 00.00 000 ET0S9 010040 000000 000000
781020 ONIIO 0.460 01.39 005 00.00 000 00.00 000 0.457 03.65 005 00.00 000 00.00 000 ET0S7 033010 000000 000000
781021 ONIIO 0.497 03.50 005 00.00 000 00.00 000 0.495 03.54 005 00.00 000 00.00 000 ET0S9 007010 000000 000000
781022 ONIIO 0.490 01.40 005 00.00 000 00.00 000 0.487 01.40 005 00.00 000 00.00 000 ET0S9 007010 000000 000000
781025 ONIMB 0.444 00.20 002 01.16 148 00.00 000 0.442 01.22 005 00.00 000 00.00 000 ET0S9 010040 000000 000000
781029 ONIIO 0.498 01.35 005 00.00 000 00.00 000 0.495 03.68 005 00.00 000 00.00 000 ET0S5 033000 000000 000000
781102 ONIIO 0.553 03.52 005 00.00 000 00.00 000 0.550 01.41 005 00.00 000 00.00 000 ET0S8 033011 000000 000000
781107 ONIIO 0.441 01.37 005 00.00 000 00.00 000 0.441 02.67 002 00.00 000 00.00 000 ET0S5 010045 000000 000000
790521 CNIIA 0.004 02.81 148 00.00 000 00.00 000 0.004 00.03 148 00.00 000 00.00 000 ET0S7 006011 000000 000000
790531 ONIIO 0.491 02.70 005 00.00 000 00.00 000 0.502 02.69 005 50.00 442 00.00 000 ET0S5 020050 000000 000000
790601 ONIIO 0.535 01.52 005 00.00 000 00.00 000 0.537 01.52 005 00.00 000 00.00 000 ET0S5 007051 000000 000000
790602 ONIIO 0.216 01.55 005 00.00 000 00.00 000 0.215 01.56 005 40.60 442 00.00 000 ET0S7 020010 000000 000000
790612 ONIMB 0.500 00.03 005 00.00 000 00.00 000 0.494 00.53 005 00.80 148 00.00 000 ET0S7 029010 012000 012000
790613 ONIMB 0.452 02.81 005 00.00 000 00.00 000 0.443 02.73 005 03.16 055 00.00 000 ET0S7 027007 015000 015000
790614 ONIMB 0.451 01.02 005 00.00 000 00.00 000 0.443 01.79 005 03.02 055 00.00 000 ET0S7 027008 015000 015000
790620 ONIIX 0.107 06.23 012 00.00 000 00.00 000 0.102 06.00 168 00.00 000 00.00 000 ET0S6 010010 000000 000000
790627 ONIIX 0.337 05.05 162 00.00 000 00.00 000 0.333 15.50 055 00.00 000 00.00 000 ET0S6 010010 000000 000000
790629 ONIIO 0.459 03.03 005 00.00 000 00.00 000 0.452 03.70 005 00.00 000 00.00 000 ET0S6 007051 000000 000000
790721 CNIIA 0.009 02.00 148 00.00 000 00.00 000 0.015 02.00 148 00.00 000 00.00 000 ET0S4 006011 000000 000000
790729 ONIIO 0.925 01.99 005 00.00 000 00.00 000 0.920 01.08 005 11.98 442 00.00 000 ET0S5 020050 000000 000000
790730 ONIIA 0.208 02.00 139 15.80 442 00.00 000 0.292 02.00 139 00.00 000 00.00 000 ET0S7 020050 000000 000000
790731 ONIIU 0.513 01.43 139 00.00 000 00.00 000 0.513 05.13 005 00.00 000 00.00 000 ET0S7 010051 000000 000000
790801 ONIIA 0.349 01.91 148 00.00 000 00.00 000 0.353 01.00 139 00.00 000 00.00 000 ET0S8 010002 000000 000000
790802 ONIIU 0.205 01.49 005 00.00 000 00.00 000 0.205 01.01 139 00.00 000 00.00 000 ET0S7 010006 000000 000000
790804 ONIIU 0.227 00.08 002 00.00 000 00.00 000 0.230 00.56 139 00.00 000 00.00 000 ET0S6 010013 000000 000000
790805 ONIIU 0.630 04.11 002 00.00 000 00.00 000 0.539 01.20 139 00.00 000 00.00 000 ET0S5 010003 000000 000000
790813 ONIIO 0.496 04.39 005 00.00 000 00.00 000 0.108 00.57 005 00.00 000 00.00 000 ET0S7 033010 000000 000000
790816 ONIIR 0.322 04.99 071 00.00 000 00.00 000 0.320 05.20 055 00.00 000 00.00 000 ET0S5 010045 000000 000000
790816 ONIMB 0.443 01.42 005 00.00 000 00.00 000 0.436 00.17 002 01.30 148 00.00 000 ET0S9 010010 000000 000000
790907 ONIMB 0.547 00.09 002 01.25 139 00.00 000 0.549 00.06 002 01.25 139 00.00 000 ET0S5 000010 012000 012000
791009 ONIIP 0.207 14.30 012 00.00 000 00.00 000 0.207 14.20 019 00.00 000 00.00 000 ET0S0 010020 000000 000000
791014 ONIIO 0.503 02.92 005 00.00 000 00.00 000 0.502 02.94 005 00.00 000 00.00 000 ET0S9 007010 000000 000000
791018 ONIIP 0.202 15.90 027 00.00 000 00.00 000 0.201 13.00 012 00.00 000 00.00 000 ET0S7 010020 000000 000000
791020 ONIIX 0.224 12.10 027 00.00 000 00.00 000 0.223 13.50 168 00.00 000 00.00 000 ET0S5 010009 000000 000000
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Table 35 cont.

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791024 ONIIO 0.456 03.55 005 00.00 000 00.00 000 0.446 03.54 005 00.00 000 00.00 000 ET0S8 007020 000000 000000
791211 ONIIX 0.239 12.50 027 00.00 000 00.00 000 0.242 14.10 150 00.00 000 00.00 000 ET0S9 010050 000000 000000
800604 ONIIX 0.176 04.80 140 00.00 000 00.00 000 0.176 03.00 160 00.00 000 00.00 000 ET0S9 010010 000000 000000
800612 ONIIX 0.221 10.90 201 00.00 000 00.00 000 0.000 00.00 000 00.00 000 00.00 000 ET0S7 010051 000000 000000
800614 ONIMB 0.210 02.25 112 00.90 093 00.00 000 0.212 01.70 112 00.00 000 00.00 000 ET0S8 027010 017000 017000
800615 ONIIO 0.213 01.22 112 00.00 000 00.00 000 0.219 00.80 112 00.00 000 00.00 000 ET0S6 033011 017000 017000
800617 ONIIO 0.192 00.50 093 00.00 000 00.00 000 0.098 01.40 093 00.00 000 00.00 000 ET0S5 033020 017000 017000
800620 ONIS  0.477 00.50 093 00.00 000 00.00 000 0.000 00.00 000 00.00 000 00.00 000 ET0S7 000050 017000 017000
800621 ONIS  0.499 01.97 112 00.00 000 00.00 000 0.000 00.00 000 00.00 000 00.00 000 ET0S6 000050 017000 017000
800708 ONIIO 0.754 02.10 002 00.00 000 00.00 000 0.754 03.23 002 00.00 000 00.00 000 ET0S5 033010 000000 000000
800709 ONIIA 0.746 01.70 196 00.00 000 00.00 000 0.751 01.50 197 00.00 000 00.00 000 ET0S5 010050 000000 000000
800715 ONIIO 0.184 01.04 112 00.00 000 00.00 000 0.188 02.60 112 00.00 000 00.00 000 ET0S6 033002 017000 017000
800716 ONIIO 0.186 04.01 093 00.00 000 00.00 000 0.188 01.97 093 00.00 000 00.00 000 ET0S9 033110 017000 017000
800717 ONIIO 0.460 02.50 093 00.00 000 00.00 000 0.466 00.90 093 00.00 000 00.00 000 ET0S9 033002 017000 017000
800725 ONIIO 0.247 01.02 112 00.00 000 00.00 000 0.252 00.94 112 00.00 000 00.00 000 ET0S7 009020 017000 017000
800730 ONIIR 0.179 03.70 055 00.00 000 00.00 000 0.178 02.23 071 00.00 000 00.00 000 ET0S7 010035 000000 000000
800801 ONIMB 0.533 00.40 002 00.23 014 00.00 000 0.551 00.46 002 00.23 014 00.00 000 ET0S9 000010 013000 013000
800808 ONIIA 0.419 01.90 140 00.00 000 00.00 000 0.419 00.85 196 00.00 000 00.00 000 ET0S9 010001 000000 000000
800809 ONIMB 0.470 40.00 150 00.00 000 00.00 000 0.467 36.46 150 01.00 139 00.00 000 ET0S7 026010 039000 039000
800811 ONIMB 0.305 03.10 055 00.00 000 00.00 000 0.310 03.14 055 01.12 162 00.00 000 ET0S4 029010 015000 015000
800812 ONIMB 0.481 00.84 139 00.00 000 00.00 000 0.484 01.00 139 01.55 162 00.00 000 ET0S4 029010 012000 012000
800813 ONIMB 0.532 22.50 160 00.00 000 00.00 000 0.253 10.46 168 00.90 139 00.00 000 ET0S8 026010 039000 039000
800814 ONIMB 0.470 00.91 002 00.29 014 00.00 000 0.466 00.95 002 00.32 014 00.00 000 ET0S6 008050 013000 013000
800826 ONIIO 0.472 01.99 002 00.00 000 00.00 000 0.464 01.00 002 00.00 000 00.00 000 ET0S8 033002 000000 000000
800827 ONIMB 0.482 02.25 055 99.99 442 00.00 000 0.491 01.91 005 99.99 442 00.00 000 ET0S8 010010 000000 000000
810615 CNIB  0.002 00.00 999 00.00 000 00.00 000 0.002 00.00 999 00.00 000 00.00 000 ET6L7 001005 000000 000000
810616 DNIB  0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 ET0L7 001010 006000 006000
810617 CNIB  0.002 00.00 999 00.00 000 00.00 000 0.002 00.00 999 00.00 000 00.00 000 ET6L7 001010 000000 000000
810618 DNIB  0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 ET0L7 001010 000000 000000
810619 ONIIO 0.500 02.00 093 00.00 000 00.00 000 0.500 01.00 093 00.00 000 00.00 000 ET6L5 033500 017000 017000
810621 ONIIO 0.500 02.00 093 00.00 000 00.00 000 0.500 01.00 093 00.00 000 00.00 000 ET4P8 033003 017000 017000
810622 ONIIO 0.700 02.00 093 00.00 000 00.00 000 0.700 01.00 093 00.00 000 00.00 000 ET5N8 033030 017000 017000
810623 ONIIO 0.500 02.00 093 00.00 000 00.00 000 0.500 01.00 093 00.00 000 00.00 000 ET7P7 033011 017000 017000
810624 ONIIO 0.430 01.58 093 00.00 000 00.00 000 0.433 01.52 005 00.00 000 00.00 000 ET6P8 010002 017000 017000
810625 ONIMC 0.200 01.60 691 00.40 093 00.00 000 0.200 02.00 691 00.00 000 00.00 000 RE6P8 023010 000000 000000
810629 ONIMC 0.200 01.30 691 00.29 055 00.00 000 0.200 01.71 691 00.00 000 00.00 000 RE6P9 023009 000000 000000
810706 ONIMC 0.200 02.00 691 00.00 000 00.00 000 0.200 02.00 691 00.00 000 00.00 000 ET4N1 008999 000000 000000
810708 ONIIO 0.500 02.00 093 00.00 000 00.00 000 0.500 02.00 002 00.00 000 00.00 000 ET4L7 010024 017000 017000
810709 ONIMC 0.500 02.00 691 00.00 000 00.00 000 0.500 01.40 691 00.60 068 00.00 000 RE5L7 023075 000000 000000
810715 ONIMB 0.300 01.40 012 00.60 005 00.00 000 0.300 00.90 012 00.42 005 00.60 055 RE4P7 024012 020000 020000
810718 TNIMB 0.300 01.40 012 00.60 005 00.00 000 0.300 00.90 012 00.42 005 00.62 068 RE5P8 024010 000000 000000
810719 SNIMB 0.300 01.40 012 00.60 005 00.00 000 0.300 00.90 012 00.42 005 00.60 068 ET5P8 024010 000000 000000
810720 ONIMC 0.500 01.40 691 00.60 068 00.00 000 0.500 01.40 691 00.60 055 00.00 000 RE4L6 010007 000000 000000
810721 ONIMC 0.300 02.00 691 00.00 000 00.00 000 0.300 01.40 691 00.00 000 00.00 000 RE4U8 033010 000000 000000
810722 ONIMC 0.300 02.00 691 00.00 000 00.00 000 0.300 01.40 691 00.60 068 00.00 000 RE4U8 023076 000000 000000
810723 ONIIU 0.500 01.50 093 00.00 000 00.00 000 0.500 01.50 139 00.00 000 00.00 000 ET4P7 010015 017000 017000
810731 ONIIA 0.500 01.50 147 00.00 000 00.00 000 0.500 01.50 146 00.00 000 00.00 000 ET5P7 010015 000000 000000
810802 CNIB  0.500 00.00 999 00.00 000 00.00 000 0.500 00.00 999 00.00 000 00.00 000 ET4U7 002999 000000 000000
810803 CNIB  0.500 00.00 999 00.00 000 00.00 000 0.500 00.00 999 00.00 000 00.00 000 ET4L4 005010 000000 000000
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Table 35 cont.

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810004 DNIB  0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 ET0L4 005010 000000 000000
810005 ONIIA 0.443 01.60 146 00.00 000 00.00 000 0.446 01.51 147 00.00 000 00.00 000 ET4S8 010002 000000 000000
810011 ONIMC 0.300 02.00 691 00.00 000 00.00 000 0.300 01.40 691 00.60 068 00.00 000 RE5L3 023010 000000 000000
810013 ONIIA 0.467 01.99 147 00.00 000 00.00 000 0.469 01.90 146 00.00 000 00.00 000 ET5S6 010010 000000 000000
810014 ONIIA 0.284 01.00 147 00.00 000 00.00 000 0.281 01.50 146 00.00 000 00.00 000 ET5S7 010009 000000 000000
810021 ONIMC 0.300 02.00 692 00.00 000 00.00 000 0.300 01.40 692 00.60 694 00.00 000 RE5L7 025051 000000 000000
810025 ONIMC 0.000 01.40 691 00.60 694 00.00 000 0.300 01.40 692 00.60 694 00.00 000 RE2L8 010011 000000 000000
810026 ONIMC 0.711 01.46 691 00.56 694 00.00 000 0.235 01.37 692 00.58 694 00.00 000 RE6S8 010010 000000 000000
810027 ONIMC 0.234 02.11 692 00.00 000 00.00 000 0.233 01.43 692 00.58 694 00.00 000 RE4S7 025010 000000 000000
810031 ONIMC 0.239 02.04 692 00.00 000 00.00 000 0.236 02.09 691 00.00 000 00.00 000 RE6S8 010010 000000 000000
810902 ONIMC 0.246 02.04 691 00.43 694 00.00 000 0.247 01.62 691 00.75 694 00.00 000 RE3S7 010010 000000 000000
810903 ONIMC 0.235 01.70 691 00.53 694 00.00 000 0.231 01.40 691 00.46 694 00.57 005 RE4S7 026010 000000 000000
810909 ONBIO 0.165 01.02 093 00.00 000 00.00 000 0.012 00.05 093 00.00 000 00.00 000 ET4S7 035301 017000 017000
810910 ONIMC 0.235 02.79 691 00.70 694 00.00 000 0.246 01.02 691 00.50 694 02.21 012 RE3S7 026010 000000 000000
810912 ONIMC 0.251 01.60 691 00.55 694 00.00 000 0.205 01.14 691 00.39 694 00.62 012 RE4S7 026010 000000 000000
810914 ONIMC 0.249 01.50 691 00.61 060 00.00 000 0.247 01.65 691 00.52 055 00.00 000 RE5S8 010009 000000 000000
810917 CNIB  0.362 00.00 999 00.00 000 00.00 000 0.363 00.00 999 00.00 000 00.00 000 ET4S9 002010 000000 000000
810918 DNIB  0.362 00.00 999 00.00 998 00.00 000 0.363 00.00 999 00.00 998 00.00 000 ET0S9 002010 000000 000000
810919 ONIMC 0.235 01.40 691 00.00 000 00.00 000 0.235 01.40 691 00.00 000 00.00 000 ET2L8 000010 000000 000000
810920 ONIMC 0.230 01,62 691 00.65 693 00.00 000 0.229 01.57 691 00.51 694 00.00 000 RE3S9 010010 000000 000000
810922 ONIMB 0.300 01.40 012 00.60 005 00.00 000 0.300 00.42 005 00.90 012 00.60 055 RE4L9 024011 000000 000000
810923 ONIMC 0.300 01.40 691 00.10 140 00.50 055 0.300 01.40 691 00.10 140 00.50 060 RE4L8 010050 000000 000000
810924 ONIMB 0.235 01.20 012 00.52 005 00.00 000 0.233 00.09 012 00.36 005 00.77 055 RE5S8 024011 000000 000000
810928 ONIIA 0.220 01.00 197 00.00 000 00.00 000 0.585 01.50 196 00.00 000 00.00 000 ET5S6 010049 000000 000000
810929 ONIMC 0.230 01.95 691 00.10 140 00.53 055 0.245 01.90 691 00.10 140 00.40 060 RE5S8 010009 000000 000000
810930 ONIMC 0.300 01.40 691 00.60 694 00.00 000 0.300 00.17 695 00.13 002 00.10 014 RE5L8 010010 000000 000000
811001 ONIIA 0.500 01.00 196 00.00 000 00.00 000 0.500 01.00 197 00.00 000 00.00 000 ET7S8 010030 000000 000000
811002 ONIIO 0.500 04.00 005 00.00 000 00.00 000 0.500 04.00 005 00.00 000 00.00 000 ET6L7 007040 000006 000000
811003 ONIMC 0.300 02.10 691 00.15 140 00.75 060 0.300 02.10 691 00.15 140 00.75 055 RE3L9 010012 000000 000000
811004 ONIMC 0.300 02.10 691 00.90 694 00.00 000 0.300 02.10 691 00.90 693 00.00 000 RE1L9 010011 000000 000000
811014 ONIMC 0.277 02.60 691 00.15 140 00.71 060 0.293 02.72 691 00.15 140 00.71 078 RE5S9 010010 000000 000000
811015 ONIMC 0.300 03.00 692 00.00 000 00.00 000 0.300 03.00 691 00.00 000 00.00 000 RE3L6 010101 000000 000000
811016 ONIMC 0.300 02.10 691 00.00 000 00.00 000 0.300 02.10 692 00.00 000 00.00 000 RE4L5 010066 000000 000000
811018 ONIIO 0.500 04.00 005 00.00 000 00.00 000 0.500 04.00 005 00.00 000 00.00 000 ET3N5 007100 000000 000000
811026 ONIIO 0.500 04.00 005 00.00 000 00.00 000 0.500 04.00 005 00.00 000 00.00 000 ET3N0 007500 000000 000000
811028 ONIMC 0.500 02.73 691 01.17 694 00.40 140 0.500 04.00 699 00.00 000 00.00 000 RE4L9 010999 000000 000000
811029 ONIMC 0.000 02.73 691 01.17 694 00.04 140 0.000 04.00 699 00.00 000 00.00 000 RE4U3 010100 000000 000000
811103 ONIMC 0.421 02.73 691 01.10 694 00.04 140 0.421 04.00 699 00.00 000 00.00 000 RE4L6 010999 000000 000000
811113 ONIMC 0.500 02.73 691 01.10 694 00.04 140 0.500 04.00 699 00.00 000 00.00 000 RE0P9 010010 000000 000000
811115 CNIB  0.333 00.00 999 00.00 000 00.00 000 0.310 00.00 999 00.00 000 00.00 000 ET4S8 005010 000000 000000
811116 DNIB  0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 ET0S8 005010 000000 000000
811118 ONIMC 0.200 02.00 691 00.00 000 00.00 000 0.200 02.00 691 00.00 000 00.00 000 ET6N1 008999 000000 000000
811122 ONIIA 0.259 00.76 140 00.00 000 00.00 000 0.263 00.01 140 00.00 000 00.00 000 ET5S8 009005 000000 000000
820413 ONIIO 0.400 04.00 005 00.00 000 00.00 000 0.400 04.00 005 00.00 000 00.00 000 ET2N2 007999 000000 000000
820520 ONIIO 0.500 04.00 005 00.00 000 00.00 000 0.500 04.00 005 00.00 000 00.00 000 ET4N2 007500 000000 000000
820602 ONIMC 0.500 01.40 691 00.36 055 00.12 060 0.500 01.40 691 00.60 068 00.00 000 RE5L7 010009 000000 000000
820606 CNIB  0.004 00.00 999 00.00 000 00.00 000 0.012 00.00 999 00.00 000 00.00 000 ET5S8 001001 000000 000000
820607 DNIB  0.000 01.00 140 00.00 998 00.00 000 0.000 01.00 140 00.00 998 00.00 000 ET0S8 001055 006000 006000
820608 ONIMC 0.281 02.26 691 00.74 065 00.00 000 0.281 02.20 691 00.70 055 00.00 000 RE6S7 010009 000000 000000
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Table 35 cont.

020609	ONIMB	0.290	01.98	012	00.64	005	00.50	068	0.284	01.96	012	00.62	005	00.53	055	RE2S7	018004	022000	022000
020614	ONIIA	0.312	03.00	148	00.00	000	00.00	000	0.300	03.06	172	00.00	000	00.00	000	ET5S7	018009	000000	000000
020615	ONIMC	0.320	03.40	691	00.00	000	00.00	000	0.312	02.54	691	00.06	693	00.00	000	RE7S8	023010	000000	000000
020616	CNIB	0.000	00.00	999	00.00	000	00.00	000	0.000	00.00	999	00.00	000	00.00	000	ET4S8	001010	000000	000000
020617	DNIB	0.500	00.00	998	00.00	000	00.00	000	0.500	00.00	998	00.00	000	00.00	000	ET0S8	002050	000000	000000
020621	ONIIO	0.320	04.00	005	03.00	442	00.00	000	0.320	04.00	005	03.00	442	00.00	000	ET6L5	007076	000000	000000
020625	ONIMC	0.617	00.55	606	00.00	000	00.00	000	0.640	00.55	606	00.00	000	00.00	000	AU6S8	009040	031000	031000
020627	CNIB	0.456	00.00	999	54.80	442	00.00	000	0.446	00.00	999	00.00	000	00.00	000	ET4S8	003011	000000	000000
020629	ONIMC	0.244	02.46	606	00.00	000	00.00	000	0.260	02.48	606	00.00	000	00.00	000	AU6S8	009040	031000	031000
020630	ONIMC	0.329	03.13	606	00.00	000	00.00	000	0.327	02.84	606	00.00	000	00.00	000	AU6S9	009040	031000	031000
020701	ONIMC	0.369	03.53	604	00.00	000	00.00	000	0.352	03.60	604	00.00	000	00.00	000	AU6S9	009040	031000	031000
020702	ONIIO	0.500	03.00	005	00.00	000	00.00	000	0.500	03.00	005	00.00	000	00.00	000	ET4L8	007020	000000	000000
020703	CNIB	0.000	00.00	999	00.45	437	00.00	000	0.000	00.00	999	00.50	437	00.00	000	ET5S8	004001	000000	000000
020704	DNIB	0.000	00.00	998	00.00	000	00.00	000	0.000	00.00	998	00.00	000	00.00	000	ET0S8	004001	000000	000000
020706	ONIMC	0.220	01.43	696	00.09	073	00.00	000	0.225	01.38	696	00.04	055	00.00	000	RE5S8	010010	000000	000000
020708	ONIMC	0.291	01.19	695	00.09	694	00.00	000	0.283	01.00	695	01.03	693	00.00	000	RE7S9	010010	000000	000000
020710	ONIMC	0.140	01.50	604	00.00	000	00.00	000	0.140	01.50	604	00.00	000	00.00	000	AU6N2	009999	031000	031000
020715	ONIMC	0.566	01.71	606	00.53	068	00.00	000	0.576	01.88	606	00.43	055	00.00	000	AU6S8	018050	031000	031000
020717	CNIIA	0.003	00.52	139	00.00	000	00.00	000	0.007	00.58	139	00.00	000	00.00	000	ET5S8	006010	000000	000000
020718	DNIIA	0.500	00.00	998	00.00	000	00.00	000	0.500	00.00	998	00.00	000	00.00	000	ET0S8	002010	000000	000000
020719	ONIMC	0.294	02.10	691	00.60	693	00.00	000	0.291	02.07	696	00.60	693	00.00	000	RE7S6	018050	000000	000000
020720	ONIMC	0.061	01.05	604	00.00	000	00.00	000	0.061	01.95	605	00.00	000	00.00	000	AU6N5	009999	031000	031000
020721	ONIMB	0.300	03.00	442	04.00	005	00.00	000	0.300	03.00	442	04.00	005	00.00	000	ET0U8	009999	000000	000000
020722	ONIMC	0.300	03.50	694	00.00	000	00.00	000	0.300	02.90	693	00.00	000	00.00	000	RE5L2	018075	000000	000000
020726	ONIMC	0.301	02.03	691	00.07	073	00.00	000	0.309	02.04	691	00.92	065	00.00	000	RE4S8	018010	000000	000000
020727	ONIMC	0.280	00.91	068	02.20	691	00.00	000	0.290	02.20	691	00.92	073	00.00	000	RE5S8	018010	000000	000000
020728	ONIMC	0.290	02.13	691	00.80	073	00.00	000	0.288	02.12	691	00.08	070	00.00	000	RE5S6	018010	000000	000000
020802	CNIB	0.389	00.00	999	00.00	000	00.00	000	0.380	00.00	999	45.40	442	00.00	000	ET4S8	003050	000000	000000
020803	ONIMC	0.456	02.45	604	00.00	000	00.00	000	0.165	01.25	605	00.00	000	00.00	000	AU8S8	033050	031000	031000
020805	ONIMC	0.300	01.55	604	00.00	000	00.00	000	0.380	01.44	605	00.00	000	00.00	000	AU6N4	009999	031000	031000
020806	ONIMC	0.374	01.30	604	00.00	000	00.00	000	0.358	01.07	605	00.00	000	00.00	000	AU7S8	009050	031000	031000
020807	ONIMC	0.293	01.40	604	00.00	000	00.00	000	0.289	01.45	605	00.00	000	00.00	000	AU5S7	009050	031000	031000
020811	ONIMC	0.300	03.00	604	00.00	000	00.00	000	0.300	03.00	605	00.00	000	00.00	000	AU7N3	009501	031000	031000
020813	ONIIO	0.500	03.00	005	00.00	000	00.00	000	0.500	03.00	005	00.00	000	00.00	000	ET5U5	034050	000000	000000
020815	ONIIO	0.500	03.00	005	00.00	000	00.00	000	0.580	03.00	005	00.00	000	00.00	000	ET3U7	007300	000000	000000
020817	ONIIO	0.300	03.00	005	00.00	000	00.00	000	0.300	03.00	005	00.00	000	00.00	000	ET3U3	007090	000000	000000
020820	CNIB	0.411	00.00	999	00.00	000	00.00	000	0.413	00.00	999	50.70	442	00.00	000	ET4S9	003001	000000	000000
020822	CNIB	0.459	00.00	999	00.00	000	00.00	000	0.457	00.00	999	40.40	442	00.00	000	ET4S8	003020	000000	000000
020823	CNIB	0.437	00.00	999	00.00	000	00.00	000	0.433	00.00	999	46.50	442	00.00	000	ET4S7	003015	000000	000000
020824	ONIIA	0.336	02.07	172	00.00	000	00.00	000	0.319	01.90	148	00.00	000	00.00	000	ET5S8	018002	000000	000000
020825	ONIIO	0.500	01.50	005	00.00	000	00.00	000	0.500	01.50	005	00.00	000	00.00	000	ET5U6	007075	000000	000000
020827	ONIIR	0.434	01.99	071	00.00	000	00.00	000	0.431	03.00	055	00.00	000	00.00	000	ET7S8	018065	000000	000000
020829	ONHIO	0.235	00.00	005	00.00	000	00.00	000	0.235	01.10	005	00.00	000	00.00	000	ET0N7	035501	000000	000000
020830	ONIIO	0.500	01.50	005	00.00	000	00.00	000	0.500	01.50	005	00.00	000	00.00	000	ET6U7	007050	000000	000000
020903	ONIIP	0.230	06.07	200	00.00	000	00.00	000	0.229	05.07	201	00.00	000	00.00	000	ET4S8	010010	000000	000000
020904	ONHIO	0.220	00.00	005	00.00	000	00.00	000	0.231	01.15	005	00.00	000	00.00	000	ET5S9	035002	013000	013000
020905	CNIB	0.497	00.00	999	00.00	000	00.00	000	0.492	00.00	999	50.00	442	00.00	000	ET3S8	003012	000000	000000
020906	ONIMB	0.456	02.33	055	00.54	071	00.00	000	0.447	01.90	055	01.05	071	00.00	000	ET5S9	010002	020000	020000
020907	ONIMB	0.471	02.40	055	00.42	071	00.00	000	0.462	02.00	055	01.02	071	00.00	000	ET6S8	010003	020000	020000

Table 35 cont.

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020908 ONIMB 0.400 03.01 055 01.70 071 00.00 000 0.475 03.00 055 00.89 071 00.00 000 ET7S7 018055 020000 020000
020909 ONIMC 0.300 02.00 691 00.00 000 00.00 000 0.300 02.00 691 00.00 000 00.00 000 ET4U7 008010 000000 000000
020910 ONBIO 0.060 00.00 005 00.00 000 00.00 000 0.255 01.10 005 00.00 000 00.00 000 ET0N6 035502 000000 000000
020911 ONIMB 0.500 01.50 005 05.00 201 00.00 000 0.500 01.50 005 00.00 000 00.00 000 ET6U5 030100 014000 014000
020912 ONIMB 0.692 01.69 005 05.00 201 00.00 000 0.364 01.69 005 00.00 000 00.00 000 ET6S8 030010 014000 014000
020913 ONBIO 0.149 00.00 005 00.00 000 00.00 000 0.321 01.09 005 00.00 000 00.00 000 ET3S9 035004 000000 000000
020914 ONIIO 0.626 01.64 005 00.00 000 00.00 000 0.614 01.64 005 00.00 000 00.00 000 ET4S7 007100 000000 000000
020916 ONIMC 0.423 02.20 691 00.92 065 00.00 000 0.426 02.20 691 00.93 068 00.00 000 RE6S8 010010 000000 000000
020917 ONIMC 0.255 02.16 604 00.00 000 00.00 000 0.254 02.42 605 00.00 000 00.00 000 AU6S7 009040 031000 031000
020918 ONIMC 0.304 02.19 691 00.91 071 00.00 000 0.386 02.20 691 00.06 068 00.00 000 RE6S7 010010 000000 000000
020921 ONIIO 0.500 01.50 005 00.00 000 00.00 000 0.500 01.50 005 00.00 000 00.00 000 ET4L2 007100 000000 000000
020923 ONIMC 0.400 02.10 691 00.90 694 00.00 000 0.400 02.10 691 00.90 693 00.00 000 RE4L9 010101 000000 000000
020924 ONIMC 0.331 02.13 696 00.00 000 00.00 000 0.331 03.06 691 00.00 000 00.00 000 ET6S7 010010 000000 000000
020925 ONIIO 0.300 03.00 005 00.00 000 00.00 000 0.300 03.00 005 00.00 000 00.00 000 ET5U7 007101 000000 000000
020928 ONIMC 0.350 03.00 691 00.00 000 00.00 000 0.350 03.00 691 00.00 000 00.00 000 ET5U8 000060 000000 000000
020929 ONIMC 0.392 01.72 604 00.00 000 00.00 000 0.390 01.74 606 00.00 000 00.00 000 AU7S8 018040 031000 031000
021001 ONIIA 0.795 01.72 197 00.00 000 00.00 000 0.778 01.50 203 00.00 000 00.00 000 ET6S7 010020 000000 000000
021003 ONIMC 0.250 02.75 696 00.00 000 00.00 000 0.240 01.56 696 00.00 000 00.00 000 RE5S9 033010 000000 000000
021006 ONIMC 0.467 01.97 606 00.00 000 00.00 000 0.466 01.96 604 00.00 000 00.00 000 AU7S9 010040 031000 031000
021008 CNIB  0.304 00.00 999 00.00 000 00.00 000 0.300 00.00 999 00.00 000 00.00 000 ET4S7 002025 000000 000000
021019 ONIIO 0.400 03.00 005 00.00 000 00.00 000 0.400 03.00 005 00.00 000 00.00 000 ET4U8 007101 000000 000000
021020 CNIB  0.000 00.00 999 00.66 437 00.00 000 0.000 00.00 999 00.53 437 00.00 000 ET3L3 004101 000000 000000
021021 DNIB  0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 ET0L3 004101 000000 000000
021022 ONIIO 0.500 04.00 005 00.00 000 00.00 000 0.500 04.00 005 00.00 000 00.00 000 ET4U3 007095 000000 000000
021027 ONIIR 0.400 04.50 055 00.00 000 00.00 000 0.399 02.78 071 00.00 000 00.00 000 ET7S8 018050 000000 000000
021028 ONIIA 0.501 01.00 196 00.00 000 00.00 000 0.487 01.00 197 00.00 000 00.00 000 ET7S8 018049 000000 000000
021101 ONIIO 0.350 04.00 005 00.00 000 00.00 000 0.350 04.00 005 00.00 000 00.00 000 ET5U2 007100 000000 000000
021102 ONIMC 0.350 03.00 691 00.00 000 00.00 000 0.350 02.10 691 00.90 693 00.00 000 RE7U8 023076 000000 000000
021106 ONIMC 0.350 03.00 691 00.00 000 00.00 000 0.350 03.00 696 00.00 000 00.00 000 RE5U9 018101 000000 000000
021108 ONIIO 0.350 04.00 005 00.00 000 00.00 000 0.350 04.00 005 00.00 000 00.00 000 ET4U8 007999 000000 000000
021111 ONIMC 0.170 02.20 691 00.90 078 00.00 000 0.171 02.52 691 00.84 073 00.00 000 RE6S8 018030 000000 000000
021112 ONIIA 0.000 00.00 000 00.00 000 00.00 000 0.250 05.00 197 00.00 000 00.00 000 ET5U7 018500 000000 000000
021115 ONIMC 0.180 02.51 696 00.00 000 00.00 000 0.183 02.74 691 00.00 000 00.00 000 RE5S9 018010 000000 000000
021123 ONIIO 0.500 04.00 005 00.00 000 00.00 000 0.500 04.00 005 00.00 000 00.00 000 ET6U2 007300 000000 000000
021207 ONIMC 0.107 02.47 691 00.90 693 00.00 000 0.186 03.49 691 00.00 000 00.00 000 RE6S9 023075 000000 000000
030610 ONIIO 0.500 03.00 005 00.00 000 00.00 000 0.500 03.00 005 00.00 000 00.00 000 ET4L5 007050 000000 000000
030612 ONIMB 0.280 02.76 695 00.00 000 00.00 000 0.280 02.76 695 00.00 000 00.00 000 RE2P8 008010 022000 022000
030614 ONBMB 0.230 01.75 695 00.05 055 00.00 000 0.000 00.00 695 00.00 055 00.00 000 ET5S9 035010 000000 000000
030617 ONIMC 0.618 01.09 604 00.00 000 00.00 000 0.629 02.40 606 00.00 000 00.00 000 AU8N4 018051 031000 031000
030618 ONIIO 0.637 01.00 005 00.00 000 00.00 000 0.538 01.00 005 00.00 000 00.00 000 ET6L5 007035 000000 000000
030620 ONIIP 0.504 01.00 202 00.00 000 00.00 000 0.509 01.00 202 00.00 000 00.00 000 ET6P4 009010 000000 000000
030623 ONIIA 0.534 01.00 197 00.00 000 00.00 000 0.530 01.00 196 00.00 000 00.00 000 ET6P9 010012 000000 000000
030625 ONIMC 0.301 03.00 696 00.00 000 00.00 000 0.292 03.00 696 00.00 000 00.00 000 RE5L5 009011 000000 000000
030627 ODCMB 0.036 00.00 695 00.00 055 00.00 000 0.280 01.83 695 00.79 055 00.00 000 ET5P8 035011 000000 000000
030628 ONIIX 0.322 03.00 204 00.00 000 00.00 000 0.319 03.00 205 00.00 000 00.00 000 ET4L7 018050 000000 000000
030629 ONIMC 0.140 02.50 604 00.00 000 00.00 000 0.155 00.80 604 00.00 000 00.00 000 AU7U5 033005 031000 031000
030702 TNIMC 0.178 01.64 604 00.00 000 00.00 000 0.184 01.70 606 00.00 000 00.00 000 AU7S8 018010 031000 031000
030703 SNIMC 0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 AU7S9 018010 031000 031000
030707 ONIIP 0.396 01.00 202 50.00 442 00.00 000 0.383 01.00 202 00.00 000 00.00 000 ET5P9 028010 012000 012000
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Table 35 cont.

030708	ONIMC	0.372	01.73	604	00.00	000	00.00	000	0.368	01.69	606	00.00	000	00.00	000	AU7S9	018035	031000	031000
030709	ONHMV	0.336	00.00	696	00.69	695	00.58	681	0.346	00.00	696	00.64	695	00.62	681	RE5S9	035030	021010	021010
030710	ONIMC	0.359	01.11	696	00.67	695	00:56	681	0.350	01.11	696	00.57	695	00.56	681	RE5L6	008010	000000	000000
030711	ONIMC	0.200	01.20	005	01.00	696	00.00	000	0.265	03.00	696	00.00	000	00.00	000	RE5P9	018010	020000	020000
030713	CNIIA	0.000	01.00	140	00.50	442	00.00	000	0.000	01.00	140	00.00	000	00.00	000	ET5L5	006010	000000	000000
030714	ONIIA	0.461	01.00	197	00.00	000	00.00	000	0.442	01.00	196	00.00	000	00.00	000	ET6P7	018002	000000	000000
030715	ONIMC	0.359	02.19	604	00.00	000	00.00	000	0.352	02.25	604	00.00	000	00.00	000	AU7S9	009035	031000	031000
030717	ONHIO	0.273	01.09	005	00.00	000	00.00	000	0.265	00.00	005	00.00	000	00.00	000	ET5S9	035003	013000	013000
030720	ONIIO	0.242	01.16	005	00.00	000	00.00	000	0.229	01.15	005	00.00	000	00.00	000	ET5L9	007035	000000	000000
030721	ONBIO	0.219	01.10	005	00.00	000	00.00	000	0.000	00.00	005	00.00	000	00.00	000	ET5S9	035005	013000	013000
030722	ONIMC	0.267	01.01	604	00.00	000	00.00	000	0.274	01.06	604	00.00	000	00.00	000	AU7N4	009501	031000	031000
030724	CNIB	0.309	00.00	999	00.00	000	00.00	000	0.406	00.00	999	00.00	000	00.00	000	ET2S8	002030	000000	000000
030725	ONIMC	0.235	02.96	600	00.00	000	00.00	000	0.222	02.84	600	00.00	000	00.00	000	AU6N7	009101	031000	031000
030726	CNIB	0.020	01.00	140	54.90	442	00.00	000	0.010	00.97	140	00.00	000	00.00	000	ET5S9	006011	006000	006000
030727	CNIB	0.464	00.00	999	48.60	442	00.00	000	0.431	00.00	999	00.00	000	00.00	000	ET3S9	003010	000000	000000
030728	ONIMC	0.294	02.50	604	00.00	000	00.00	000	0.291	02.52	604	00.00	000	00.00	000	AU8N9	009036	031000	031000
030729	ODIIO	0.217	01.09	005	00.00	000	00.00	000	0.215	01.09	005	00.00	000	00.00	000	ET5S9	035001	000000	000000
030731	ONBIO	0.217	01.09	005	00.00	000	00.00	000	0.004	00.00	005	00.00	000	00.00	000	ET5S9	035006	013000	013000
030801	ONIIR	0.395	04.59	055	00.00	000	00.00	000	0.372	02.62	071	00.00	000	00.00	000	ET8S8	018001	000000	000000
030804	CNIB	0.029	00.95	140	50.00	442	00.00	000	0.023	00.95	140	00.00	000	00.00	000	ET6S8	006050	006000	006000
030806	CNIB	0.399	00.00	999	50.00	442	00.00	000	0.374	00.00	999	00.00	000	00.00	000	ET3S9	003040	000000	000000
030808	ONIIR	0.434	06.00	071	00.00	000	00.00	000	0.421	09.00	055	00.00	000	00.00	000	ET7L5	018045	000000	000000
030809	ONIIR	0.347	04.00	070	00.00	000	00.00	000	0.334	04.00	004	00.00	000	00.00	000	ET9L5	018006	000000	000000
030811	ONIMC	0.223	02.16	606	00.00	000	00.00	000	0.218	00.60	606	00.00	000	00.00	000	AU8S9	033004	031000	031000
030813	ONIIO	0.220	01.00	005	00.00	000	00.00	000	0.212	00.70	005	00.00	000	00.00	000	RE6S8	030050	040000	040000
030814	CNIB	0.000	00.00	999	00.00	000	00.00	000	0.000	00.00	999	00.00	000	00.00	000	ET4S9	004010	000000	000000
030815	DNIB	0.000	00.00	998	00.00	000	00.00	000	0.000	00.00	998	00.00	000	00.00	000	ET4S9	004010	000000	000000
030818	ODCMB	0.280	00.42	005	01.41	012	00.79	055	0.280	00.42	005	01.41	012	00.79	055	RE7P7	035013	000000	000000
030819	ONIIP	0.300	04.62	017	00.00	000	00.00	000	0.375	04.01	002	00.00	000	00.00	000	ET8P8	018001	000000	000000
030822	ONBMV	0.212	00.49	695	00.00	696	00.56	681	0.017	00.49	695	00.00	696	00.55	681	RE9S9	035032	021000	021000
030824	CNIB	0.000	00.24	000	00.00	000	00.00	000	0.000	00.24	000	00.00	000	00.00	000	ET2P5	004030	000000	000000
030825	CNIB	0.000	01.00	140	50.00	442	00.00	000	0.000	01.00	140	00.00	000	00.00	000	ET6P7	006015	006000	006000
030826	ODCMB	0.310	00.70	055	00.42	005	01.40	012	0.110	00.00	055	00.00	005	00.00	012	ET9P9	035012	000000	000000
030902	ONIMC	0.276	03.00	604	00.00	000	00.00	000	0.278	02.40	609	00.00	000	00.00	000	AU9N4	018101	031000	031000
030905	ONIIO	0.500	01.50	005	00.00	000	00.00	000	0.500	01.50	005	00.00	000	00.00	000	ET6N5	007101	000000	000000
030906	ONIMC	0.244	02.02	691	00.00	000	00.00	000	0.230	01.03	691	00.60	040	00.00	000	RE7L7	030010	000000	000000
030907	ONIIO	0.500	01.50	005	00.00	000	00.00	000	0.500	01.50	005	00.00	000	00.00	000	ET6L7	007050	000000	000000
030909	ONIMC	0.296	02.00	604	00.00	000	00.00	000	0.298	02.06	609	00.00	000	00.00	000	AU9U7	018100	031000	031000
030912	ONCMC	0.334	01.00	691	00.00	683	00.00	685	0.335	00.50	691	00.00	683	00.00	685	RE8S9	035021	032000	032000
030916	ONIMB	0.228	00.43	002	01.57	010	01.00	005	0.208	00.84	002	01.02	010	01.04	005	RE7P5	018010	020000	020000
030918	ONIIO	0.440	01.50	005	00.00	000	00.00	000	0.440	01.50	005	00.00	000	00.00	000	ET5P8	007011	000000	000000
030920	ONIMC	0.250	02.94	604	00.00	000	00.00	000	0.249	02.40	610	00.00	000	00.00	000	AU9N4	018100	031000	031000
030921	CNIB	0.000	00.00	999	00.00	000	00.00	000	0.000	00.00	999	00.00	000	00.00	000	ET5P7	001040	000000	000000
030923	ONIIO	0.413	01.50	010	00.00	000	00.00	000	0.376	01.50	005	00.00	000	00.00	000	RE6P7	018025	000000	000000
030925	ONIIO	0.500	01.50	010	00.00	000	00.00	000	0.500	03.00	010	00.00	000	00.00	000	ET5P7	033002	000000	000000
030927	ONIIO	0.473	01.50	010	00.00	000	00.00	000	0.440	01.50	014	00.00	000	00.00	000	RE5P9	018026	000000	000000
031002	ONIIO	0.456	03.31	010	00.00	000	00.00	000	0.430	02.90	005	00.00	000	00.00	000	ET5L7	018020	013000	013000
031004	ONIMC	0.254	02.59	604	00.00	000	00.00	000	0.251	02.19	610	00.00	000	00.00	000	AU8S9	018002	031000	031000
031006	ODIMC	0.369	02.10	691	00.85	684	00.00	000	0.366	02.10	691	00.83	684	00.00	000	ET8S9	035020	000000	000000

Table 35 cont.

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831007 ONIMC 0.334 01.89 691 00.75 693 00.00 000 0.345 02.69 609 00.00 000 00.00 000 AU8S0 018002 000000 000000
831014 ONI10 0.277 02.50 006 00.00 000 00.00 000 0.274 02.50 005 00.00 000 00.00 000 ET7L5 007050 000000 000000
831015 ONIMB 0.481 01.13 005 00.44 002 01.60 010 0.497 01.00 005 00.00 002 01.10 010 RE5P8 010010 020000 020000
831017 ONHMV 0.492 01.12 005 01.26 602 00.00 685 0.456 00.00 005 01.21 602 02.01 605 RE6S8 035031 021000 021000
831019 ONIMC 0.834 00.35 604 00.00 000 00.00 000 0.836 00.35 606 00.00 000 00.00 000 AU8U7 018100 031000 031000
831024 CNIB  0.000 00.00 999 00.00 000 00.00 000 0.000 00.00 999 00.00 000 00.00 000 ET3P8 004040 000000 000000
831025 DNIB  0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 ET3P8 004040 000000 000000
831028 ONIMC 0.279 02.40 606 00.00 000 00.00 000 0.258 02.37 604 00.00 000 00.00 000 AU9U5 010100 031000 031000
831102 TNIMC 0.273 01.66 606 00.00 000 00.00 000 0.272 01.50 604 00.00 000 00.00 000 AU9U7 010100 031000 031000
831103 SNIMC 0.000 00.00 998 00.00 000 00.00 000 0.000 00.00 998 00.00 000 00.00 000 AU9U8 010100 031000 031000
831111 CNIB  0.600 50.00 442 00.00 000 00.00 000 0.600 00.00 000 00.00 000 00.00 000 ET3U8 003020 000000 000000
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